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BISON

A FORTRAN Computer System for the Calculation of Analytic Self-consistent-field Wavefunctions, Properties, and Charge Densities for Diatomic Molecules

Part 1. User's Manual and General Program Description

by

Arnold C. Wahl, P. J. Bertoncini, K. Kaiser,
and Robert H. Land

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January 1968

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ABSTRACT

Techniques and a new computer program developed by the authors for obtaining self-consistent-field (SCF) wavefunctions and properties [very close to the Hartree-Fock (HF) limit] via the Roothaan Expansion Method for heteropolar or homopolar diatomic molecules containing atoms from rows 1 through 5 of the periodic table are discussed.

The computer program, which is written entirely in FORTRAN, evaluates all necessary integrals, performs the SCF procedure and then computes charge-density contours and a variety of molecular properties from the resulting SCF wavefunction. The limitations on the quantum numbers of the Slater-type orbital (STO) basis are $1 \leq n \leq 8$; $0 \leq \ell \leq n - 1$; $-\ell \leq m \leq \ell$; a maximum of $1\frac{1}{2}$ million supermatrix elements are permitted which allows accurate SCF calculations on very large diatomic systems. Typical results of recent extended basis-set calculations for the alkali halide NaCl, which illustrate program usage, are presented.

I. INTRODUCTION

It is becoming increasingly clear that with the advent of larger and more powerful computers, rapid strides can be and are being made into previously inaccessible areas of molecular quantum mechanics. However, in order to take the fullest advantage of the meteoric progress of present-day computing machines, a great deal of effort and long-range planning must go into the design and construction of any large computer program. Further, it is mandatory that these "production" programs be modular, cumulative, machine transferable, and capable of continuous growth and revision. In order to achieve these goals realistically, a vast and well-integrated working library of computer programs must be developed in a compiler language which survives machine obsolescence.

With these principles in mind, we have developed a modular, flexible, and capable computer program for solving the Hartree-Fock equations for diatomic molecules by means of the Roothaan Expansion Method. This program is coded entirely in FORTRAN, and represents a significant advance in technique and capacity over our previous machine-language programs.¹

In this paper we describe the use of the program, and the mathematical and data-processing techniques employed in it. Some typical results obtained with the program are given.

II. THEORY AND TECHNIQUES

A. The Hartree-Fock-Roothaan Scheme

The molecular orbital model as introduced by Mulliken and Hund underlies all of present-day chemistry. Mathematically the "best" molecular orbitals when judged in terms of the total energy of the system are obtained through the Hartree-Fock equations,

$$F\varphi_i = \epsilon_i\varphi_i, \quad (1)$$

where the φ_i 's are the orbitals of the system. All orbitals φ_i contribute to the Fock operator F which represents the effective Hamiltonian of this orbital model. Equation (1) is thus a psuedo-eigenvalue equation which must be solved iteratively.

For atoms, direct numerical solution of the Hartree-Fock equations can be achieved; however, an alternative method for obtaining the orbitals φ_i has been developed by Roothaan.² In the scheme now known as the Roothaan Expansion Method the orbitals φ_i are expanded in terms of some suitable but finite set of functions,

$$\varphi_i = \sum_p C_{ip} \chi_p \quad (2)$$

The Hartree-Fock equations then become a well-organized problem in matrix algebra.

For molecules the expansion method is at present the most practical and widely used means of obtaining the molecular orbitals φ_i .¹

Roothaan and Bagus have described this scheme in general for atoms; however, their formalism as far as the SCF equations are concerned is equally suitable for molecules, and we have adopted it. Thus the equations

solved in our program are as follows. The molecular orbitals are expanded in term of some basis set

$$\varphi_{i\lambda} = \sum_p C_{i\lambda p} \chi_{p\lambda\alpha}, \quad (3)$$

where λ is the symmetry species and α the subspecies, both introduced for convenience.¹⁻³ From the coefficients $C_{i\lambda p}$ a set of density matrices are defined for each shell $i\lambda$ occupied by $N_{i\lambda}$ electrons:

$$D_{i\lambda} = N_{i\lambda} \xi_{i\lambda}^\dagger \xi_{i\lambda}. \quad (4)$$

From these closed-shell, open-shell, and total-density matrices are defined as

$$\left. \begin{aligned} D_{C\lambda} &= \sum_{i \in \text{closed}} D_{i\lambda} \\ D_{O\lambda} &= \sum_{i \in \text{open}} D_{i\lambda} \\ D_{T\lambda} &= D_{C\lambda} + D_{O\lambda} \end{aligned} \right\}. \quad (5)$$

The equation for the total energy is the remarkably compact

$$E = H^\dagger D_T + \frac{1}{2} D_T^\dagger P D_T - \frac{1}{2} D_O^\dagger Q D_O. \quad (6)$$

where the H , D_T , and D_O matrices are considered to be supervectors, H being the collection of one-electron integrals over the basis. P and Q are supermatrices which are ordered collections of all necessary two-electron integrals over the basis set. (These integrals, which represent the most time-consuming part of the calculation, are discussed in Sect. F.)

When the variational principle is applied to equation (6), two SCF equations are obtained, one for the open shells and one for the closed shells:

$$\begin{aligned} F_C \xi &= \epsilon S_C \xi; \\ F_O \xi &= \epsilon S_O \xi; \end{aligned} \quad (7)$$

where

$$\begin{aligned} F_C &= H + P + R_O; \\ F_O &= H + P - Q + R_C; \end{aligned} \quad (8)$$

(Contd.)

$$P = p D_T;$$

$$Q = q D_O;$$

$$R_{c\lambda} = [N_{c\lambda}/(N_{c\lambda} - N_{o\lambda})] \sum_{i \in \text{closed}} [S_{i\lambda} q_{i\lambda}^+ + q_{i\lambda} S_{i\lambda}^+];$$

$$R_{o\lambda} = [N_{o\lambda}/(N_{c\lambda} - N_{o\lambda})] \sum_{i \in \text{open}} [S_{i\lambda} q_{i\lambda}^+ + q_{i\lambda} S_{i\lambda}^+];$$

$$S_{i\lambda} = S_{\lambda} \xi_{i\lambda};$$

$$q_{i\lambda} = Q_{\lambda} \xi_{i\lambda}.$$

(Contd.)

(8)

As is, of course, obvious, equations (7) must be solved iteratively with the new F_c and F_o constructed at each iteration. Convergence has been achieved when all vectors $\xi_{i\lambda}$ agree between two iterations. (See Sect. II.F for the definition of H, S, P and Q for diatomic molecules.)

B. The Solution of $F_c = \epsilon S_c$

We solve the general eigenvalue problem

$$F_c = \epsilon S_c \quad (9)$$

as follows.

We diagonalize S such that

$$S = U^{-1} S_D U.$$

Then

$$F_c = \epsilon U^{-1} S_D U c. \quad (10)$$

The vector y is then defined as

$$y = S_D^{1/2} U c.$$

Then

$$F S_D^{-1/2} U^{-1} y = \epsilon U^{-1} S_D^{1/2} y. \quad (11)$$

We multiply from the left by $U S_D^{-1/2}$:

$$U S_D^{-1/2} F S_D^{-1/2} U^{-1} y = \epsilon y.$$

We then solve this new eigenvalue problem:

$$M y = \epsilon y \quad (12)$$

using the Givens method⁴ and transform the $\tilde{y}$'s back into the original space of $\tilde{c}$ to give

$$\tilde{c} = S^{-1/2}U^{-1}\tilde{y}. \quad (13)$$

We of course also get all virtual orbitals by this process and can converge upon selected sets of excited orbitals as described in the input section. We have found an accuracy of 8-10 significant figures in the eigenvalues and vectors. It is important to note that this method of solution is quite simple and general provided that S is positive definite. The initial diagonalization of S to obtain U and S_D need only be done once for a given basis; thus only one diagonalization is done for subsequent iterations.

C. Iterations and Extrapolations

Often straight iterations will lead to convergence; however, cases do arise which are either very slowly convergent or divergent. For these cases some extrapolation scheme is required. We have incorporated Hartree's method⁵ in our program, namely,

$$C_p = (C_{i+2,p}C_{i,p} - C_{i+1,p}^2)/(C_{i+2,p} - 2C_{i+1,p} + C_{i,p}), \quad (14)$$

in which C_p represent the extrapolated value of the p^{th} component of any vector and the indices i , $i+1$, and $i+2$ number the vectors obtained from 2 successive iterations.

In the program we allow a total of 100 iterations; these may be divided between initial $2N$ iterations and $100 - 2N$ extrapolations at the option of the user.

D. The Handling of the Supermatrices

A novel aspect of our computer program is that the supermatrices P and Q are constructed and stored row by row on peripheral devices.* This permits much larger basis sets than those feasible for a core-bound program. By buffering, namely, reading in and out information while performing useful computations, we have achieved adequate program speed in spite of the slowness of the peripherals. During the SCF processes all contractions necessary to form the Fock matrices (equations 8) are performed directly from peripherals. This feature has enabled us to calculate SCF solutions for previously inaccessible molecules.

E. Units, Coordinate Systems, and Basis Functions

(1) The Atomic Units advocated by Shull and Hall⁶ are used. In this system the unit of length is the Bohr (0.52917 Å), the unit of energy the Hartree (27.20974 eV) and the unit of charge that of the electron, e^- .

*Tapes on CDC-3600, disks on IBM-360/75.

(2) Coordinate Systems (see Fig. 1)Prolate spheroidal

$$\xi = \frac{r_a + r_b}{R}; \quad \eta = \frac{r_a - r_b}{R}; \quad \varphi = \varphi_a = \varphi_b. \quad (15)$$

Spherical on either center $\underline{a}$ or $\underline{b}$

$$r_a \text{ or } r_b; \quad \theta_a \text{ or } \theta_b; \quad \varphi_a \text{ or } \varphi_b.$$

Fig. 1. The Coordinate System

In the integral evaluation, depending on the type of integral being computed, the coordinate system may be Cartesian, spherical, or prolate spheroidal. An extensive discussion of these coordinates is given in Ref. 7.

(3) Basis Functions. The basis function used for expressing the molecular orbitals in the program are the normalized Slater-type Orbitals (STO's) centered on either nucleus $\underline{a}$ or $\underline{b}$ and defined as

$$\chi_{n\ell m} = (2\zeta)^{n+1/2} [(2n)!]^{-1/2} r^{n-1} e^{-\zeta r} Y_{\ell m}(\theta, \varphi), \quad (16)$$

where $Y_{\ell m}(\theta, \varphi)$ are the normalized, complex spherical harmonics defined as

$$Y_{\ell m}(\theta, \varphi) = \Phi_m(\varphi) P_{\ell m}(\cos \theta) \quad (17)$$

and

$$\Phi_m(\varphi) = (2\pi)^{-1/2} e^{im\varphi},$$

and where $P_{\ell m}$ are the normalized Legendre polynomials of the first kind. A χ is completely defined by specifying the quantum numbers n , ℓ , m , the scaling factor zeta (ζ), and the center on which the function "sits." The limitations on the STO'S are

$$1 < n \leq 8;$$

$$\ell \leq \{n - 1\};$$

$$|m| \leq \ell;$$

$$0.01 < \zeta < 100.$$

(18)

F. The Evaluation of the Matrices and Supermatrices

By far the most time-consuming and difficult part of the diatomic calculation is the accurate evaluation of the numerous integrals which occur over the basis functions. We have used a combination of analytic and numeric techniques described previously^{1,7} which leads to a reliable and efficient evaluation of all the molecular integrals in question. Below we summarize these methods and present the working computational formulas.

1. The Matrices S, U, and T

The H matrix is defined as

$$H = T - U. \quad (19)$$

The necessary one-electron integrals for diatomic molecules are thus collected in the overlap matrix,

$$S_{\lambda p q} = \langle \chi_{\lambda p \alpha} | \chi_{\lambda q \alpha} \rangle.$$

The nuclear attraction matrix

$$U_{\lambda p q} = \sum_i \langle \chi_{\lambda p \alpha} | \frac{Z_i}{r_i} | \chi_{\lambda q \alpha} \rangle \quad (20)$$

and the kinetic energy matrix

$$T_{\lambda p q} = -1/2 \langle \chi_{\lambda p \alpha} | \nabla^2 | \chi_{\lambda q \alpha} \rangle,$$

where each of the basis functions $\chi_{\lambda p \alpha}$ and $\chi_{\lambda q \alpha}$ can be centered on either center a or b of the system, Z_i is the charge of, and r_i the distance from, nucleus i . In our current program we have adopted a unified numerical approach to these integrals. We have resorted to this method to avoid the complicated and clumsy tables of coefficients⁷ necessary to compute efficiently the two-center one-electron integrals and because this very simple numerical approach leads to an insignificant increase in overall computation time. Thus we first analytically integrate over the angle φ to obtain the existence condition

$$m_{\lambda p} = m_{\lambda q};$$

then we define the charge distribution,

$$\Omega'_{\lambda pq} = (2\xi_{\lambda p})^{n_{\lambda p}+1/2} (2\xi_{\lambda q})^{n_{\lambda q}+1/2} [(2n_{\lambda p})!(2n_{\lambda q})!]^{-1/2} r^{n_{\lambda p}-1} r^{n_{\lambda q}-1} e^{-\xi_{\lambda p} r_{\lambda p} - \xi_{\lambda q} r_{\lambda q}} p_{\ell_{\lambda p} m_{\lambda p}}(\cos \theta_{\lambda p}) p_{\ell_{\lambda q} m_{\lambda q}}(\cos \theta_{\lambda q}), \quad (21)$$

which may be one- or two-center distributions depending upon the reference center of functions λp and λq .¹

We integrate this charge distribution multiplied by the appropriate one-electron operator numerically over a set of points determined by crossed gaussian grids on the prolate spherical coordinates ξ and η . Thus

$$\begin{aligned} S_{\lambda pq} &= \sum_r^N \sum_s^{N'} \tilde{W}_{rs} \Omega_{\lambda pq}(\xi_r, \eta_s); \\ U_{\lambda pq} &= \sum_i^N \sum_r^N \sum_s^{N'} \tilde{W}_{rs} \Omega_{\lambda pq}(\xi_r, \eta_s) \frac{Z_i}{r_{rs}}; \\ T_{\lambda pq} &= \sum_r^N \sum_s^{N'} \tilde{W}_{rs} \left\{ \xi_{\lambda q}^2 \Omega_{\lambda pq}(\xi_r, \eta_s) - 2n_{\lambda q} \xi_{\lambda q} \frac{1}{r_{rs}} \Omega_{\lambda pq}(\xi_r, \eta_s) \right. \\ &\quad \left. + (n_{\lambda p} + \ell_{\lambda q})(n_{\lambda q} - \ell_{\lambda q} - 1) \frac{1}{r_{rs}^2} \Omega_{\lambda pq}(\xi_r, \eta_s) \right\}, \end{aligned} \quad (22)$$

where

$$r_{rs} = (\xi_r \pm \eta_s) \frac{R}{2}$$

and the transformation used to map ξ into the finite domain^{1,7} is

$$\xi_r = \frac{1 + \beta}{1 - \beta t_r} \quad (23)$$

with

$$-1 \leq t \leq 1.$$

The parameter β truncates the ξ integration within a physically significant region of space.¹ The ξ_r 's and η 's are the normal gaussian points, namely, the zero's of the Legendre polynomials. The $\tilde{W}_{rs}$ represent the product of the gaussian weight factors W_r and W_s for the ξ and η integration, the

prolate spheroidal volume element, and the transformation weight. Thus

$$\tilde{W}_{rs} = W_r W_s (1/2R)^3 [\beta/(\beta+1)] \xi_r^2 (\xi_r^2 - \eta_s^2). \quad (24)$$

We have used these techniques in earlier work to evaluate^{1,8} a variety of one-electron properties and found them very satisfactory. In our present program up to 100 gaussian points are permitted on either ξ or η , which allows adequate accuracy of the computed integral (up to 9-10 significant figures).

2. The Supermatrices P and Q

The supermatrices P and Q are defined in the program as

$$\left. \begin{aligned} P_{\lambda p q \mu r s} &= J_{\lambda p q \mu r s} - 1/4 [\kappa_{\lambda p q \mu r s}^+ + \kappa_{\lambda p q \mu r s}^-] \\ \text{and} \\ Q_{\lambda p q \mu r s} &= A_{\lambda \mu} J_{\lambda p q \mu r s} + B_{\lambda \mu} \kappa_{\lambda p q \mu r s}^+ + C_{\lambda \mu} \kappa_{\lambda p q \mu r s}^- \end{aligned} \right\} \quad (25)$$

where

$$\left. \begin{aligned} J_{\lambda p q \mu r s} &= (d_\lambda d_\mu)^{-1} \sum_{\alpha \beta} \iint \chi_{p\lambda\alpha}(1) \chi_{r\mu\beta}(2) (1/r_{12}) \\ &\quad \chi_{q\lambda\alpha}(1) \chi_{s\mu\beta}(2) dV_1 dV_2; \\ \kappa_{\lambda p q \mu r s}^+ &= \iint \chi_{p\lambda m\lambda}(1) \chi_{s\mu m\mu}^*(2) (1/r_{12}) \chi_{r\mu m\mu}(1) \chi_{q\lambda m\lambda}(2) dV_1 dV_2; \\ \kappa_{\lambda p q \mu r s}^- &= \iint \chi_{p\lambda m\lambda}(1) \chi_{s\mu \bar{m}\mu}^*(2) (1/r_{12}) \chi_{r\mu \bar{m}\mu}(1) \chi_{q\lambda m\lambda}(2) dV_1 dV_2 \end{aligned} \right\} \quad (26)$$

and d_λ is the dimension of representation λ .

The quantities $A_{\lambda\mu}$, $B_{\lambda\mu}$, and $C_{\lambda\mu}$ are constants characteristic of the open shell structure of the molecule and are tabulated in Table 3a. $m\mu$ is the absolute value of the projection of angular momentum characteristic of symmetry μ and $\bar{m}\mu = -m\mu$. We have found it convenient to keep κ^+ and κ^- separate, which permits a wider class of open shells and allows greater flexibility in multiconfiguration SCF calculations as discussed elsewhere.⁹ Each of the four basis functions involved in the J and $\kappa^\pm$ supermatrix elements may "sit" on either of the two centers a or b of the system. This gives rise to four types of two-electron integrals, namely:

$$\left. \begin{aligned}
 &\text{a. } \underline{\text{one-center}} \\
 &\iint \chi_a^*(1) \chi_a^{*'}(2) (1/r_{12}) \chi_a''(1) \chi_a'''(2) dV_1 dV_2; \\
 &\text{b. } \underline{\text{two-center Coulomb}} \\
 &\iint \chi_a^*(1) \chi_b^*(2) (1/r_{12}) \chi_a'(1) \chi_b'(2) dV_1 dV_2; \\
 &\text{c. } \underline{\text{two-center hybrid}} \\
 &\iint \chi_a^*(1) \chi_a^{*'}(2) (1/r_{12}) \chi_a''(1) \chi_b(2) dV_1 dV_2; \\
 &\text{d. } \underline{\text{two-center exchange}} \\
 &\iint \chi_a^*(1) \chi_a^{*'}(2) (1/r_{12}) \chi_b(1) \chi_b'(2) dV_1 dV_2.
 \end{aligned} \right\} \quad (27)$$

(a) The one-center integrals are easily evaluated analytically by conventional techniques used in atomic calculations. The angles θ_1 , θ_2 , φ_1 , and φ_2 may be integrated analytically to yield products of Clebsch-Gordon coefficients⁷ and a double radial integral.³ After performing the angular integration the working expression is

$$I = \sum_{\lambda} \left[\begin{matrix} l+l'' \\ l'+l''' \end{matrix} \right]_{\min} T_{\lambda}(l, l''; m, m'') T_{\lambda}(l', l'''; m', m''') K_{\lambda}(n, \zeta, n', \zeta', n'', \zeta'', n''', \zeta''')$$

$$\lambda = \left[\begin{matrix} [l - l''] \\ [l' - l'''] \\ [m - m''] \end{matrix} \right]_{\max}$$

where

$$T_{\lambda}(l, l''; m, m'') = (2l+1)(2l''+1)/(2\lambda+1) C(l, l'', \lambda; 000) C(l, l'', \lambda; m, m'', m - m'')$$

and

$$K_{\lambda}(p, q, r, s) = K_{\lambda pqrs}^V$$

of Ref. 3 where $p \rightarrow \frac{n}{\zeta}$, $q \rightarrow \frac{n''}{\zeta''}$, $r \rightarrow \frac{n'}{\zeta'}$, $s \rightarrow \frac{n'''}{\zeta'''}$.

(b, c) The two-center Coulomb and Hybrid integrals are evaluated by a combination of analytic and numerical techniques,^{1,7} which reduces the integral to a final two-dimensional integration over the prolate spheroidal coordinates ξ and η , the integrands being the electrostatic potential due to the one-center charge distribution and the remaining one- or two-center charge distribution.¹ The working expression is

$$\iint \Omega_a(1) 1/r_{12} \Omega_{ab}(2) dV_1 dV_2 = \delta(m - m'_a, m''_b - m_b) \times \sum_{r=1}^N \sum_{s=1}^{N'} [W_r W_s (1/2R)^3 \{\beta/(\beta+1)\} \xi_r^2 (\xi_r^2 - \eta_s^2) U_a(\xi_r, \eta_s) \Omega_{ab}(\xi_r, \eta_s)], \quad (28)$$

where r and s refer to points in a crossed gaussian integration over the prolate spheroidal coordinates ξ and η , and β is defined in equation (23).

$U_a(\xi_r, \eta_s)$, the electrostatic potential due to electron 1, has been evaluated by analytic integration^{1,7} over the coordinates of electron 1 and is given by

$$U_a(\xi, \eta) = [1/2R(\xi + \eta)]^{n_a + n'_a} \sum_{\lambda_{\min}}^{\lambda_{\max}} T_\lambda P_{\lambda, m_a - m_a} \frac{1 + \xi\eta}{(\xi + \eta)} \times \left[E_{n_a + n'_a + \lambda} [R(\xi_a + \xi'_a)(\xi + \eta)/2] \right] + A_{n_a + n'_a - \lambda - 1} [R(\xi_a + \xi'_a)(\xi + \eta)/2]$$

and

$$\Omega_{ab}(\xi, \eta) = \chi_a(\xi, \eta) \chi_b(\xi, \eta) (2\pi) e^{-i(m''_b - m_b) \varphi},$$

which is just the ξ, η dependence of the charge distribution of electron 2.^{1,7} The auxiliary functions and expanded form of $\Omega(\xi, \eta)$ are defined in Ref. 7.

(d) The two-center exchange integrals are evaluated by expanding both two-center charge distributions in prolate spheroidal coordinates, introducing the Neumann expansion for $1/r_{12}$, integrating analytically over $\varphi_1, \varphi_2, \eta_1$, and η_2 , and performing a final double numerical integration over ξ_1 and ξ_2 . The basic working formula is

$$\int \Omega_{ab}(1) 1/r_{12} \Omega'_{ab}(2) dV = \frac{4}{R} \kappa_{ab} \kappa'_{ab} \delta(M, M') \sum_{\lambda=M}^{\infty} I_\lambda, \quad (30)$$

where

$$I_\lambda = \int_1^\infty \frac{d\xi}{(\xi^2 - 1)} [P_\lambda^M(\xi)]^2 F_\lambda^M(\xi; \tau, \rho) F_\lambda^{M'}(\xi; \tau', \rho');$$

$$F_\lambda^M(\xi; \tau, \rho) = \int_1^\xi dx P_\lambda^M(x) (x^2 - 1)^{M/2} \times \sum_{j=0}^{N-M} B_{j\lambda}^M(-\rho\tau) \sum_{n=0}^{N-M} a_{nj} x^n \exp(-\rho x);$$

κ_{ab} are normalization factors and $M = m_a - m_b$.

A Simpson rule integration is performed over 5. The same set of points are appropriate for evaluating the integrals over x . This resulting interlaced numerical integration is very efficient.^{1,7} In fact, the exchange integrals are evaluated more rapidly than either the Coulomb or hybrid integrals. The auxiliary functions $B_{j\lambda}^M$ and expansion coefficients a_{nj} are defined in Ref. 7.

The above summary of the methods used to evaluate the two-electron integrals is only intended to clarify program usage. For a detailed treatment of these methods and the economics achievable with them, the user should rely heavily on Refs. 1 and 7, and on a companion report describing the FORTTRAN Structure of the program.¹⁰

3. The Point Charge Environment Matrix L

Provision has been made in the program for the solution of the SCF equations for the molecule in the presence of an external set of point charges. This gives rise to the modified SCF equations

$$F_{c\tilde{c}} = eS_{c\tilde{c}}$$

$$F_{0\tilde{c}} = eS_{0\tilde{c}}$$

$$F_c = H + L + PD_T - QD_0$$

$$F_0 = H + L + QD_0$$

$$E = H^+D_T + L^+D_T + \frac{1}{2}D_T^+PD_T - \frac{1}{2}D_0^+QD_0$$

where H , P , Q , and D_T and D_0 are as defined in Sect. II and L is the external field matrix defined by

$$L_{\lambda p q} = \sum_k Z_k \left\langle \chi_{\lambda p} \left| \frac{1}{r_k} \right| \chi_{\lambda q} \right\rangle$$

where Z_k is the point charge at position r_k (see Fig. 2). The integrals $\left\langle \chi_{\lambda p} \left| \frac{1}{r_k} \right| \chi_{\lambda q} \right\rangle$ fall into three distinct classes: 1) the one-center Coulomb, 2) two-center Coulomb, and 3) three-center nuclear attraction. The first type presents no difficulty. The methods we have used for types 2 and 3 have been described recently.¹⁰ Currently the matrix L is loaded as optional input to the program.

Fig. 2. Point Charge Geometry

G. The Calculation of Molecular Properties

A variety of molecular properties can be computed at the user's option from the

SCF wavefunction. Currently the properties considered are: $\sin^2 \frac{\theta_a}{r_a}$, $\cos^2 \frac{\theta_a}{r_a}$, $3z_a^2 - r_a^2$, $\frac{1}{r_a}$, r_a^2 , z_a^2 , $\sin^2 \frac{\theta_b}{r_b}$, $\cos^2 \frac{\theta_b}{r_b}$, $3z_b^2 - r_b^2$, $\frac{1}{r_b}$, z_b^2 , ξ , η , x , and z .

Again a unified numerical approach is taken in the computation of these operators. Thus

$$\langle M \rangle = \sum_r^N \sum_s^{N'} \tilde{W}_{rs} \tilde{M}_{rs} \Omega_{\lambda pq}(\xi_r, \eta_s)$$

where M is the value of the property operator at the points r and s in space and the other quantities are weight factors and charge distributions are defined in Sect. II-F-1.

H. The Plotting of Charge Density Contours

The program upon request will generate and plot contour diagrams of the orbital and total density of the molecule. An interesting feature of this process is that the contours are hunted out and plotted automatically and appear on 35-mm film as computer output or on an off-line CalComp. plotter. This contour hunting and drawing process has been described recently.¹² Such contour diagrams are presented for NaCl in Figs. 3a-3l.

III. PROGRAM DESIGN AND SPECIAL FEATURES

A. Modularity

The program has been designed in a modular fashion with only the minimum information linking self-contained sections. This permits the addition of new sections and revision of existing ones with essentially no changes of the uninvolved modules. For example, the *J*, *K*, the density-contour drawing, and the one-electron and molecular-properties overlays can be used equally well as independent programs. In fact, the program has been frequently used as a package to generate integrals.

B. Interruptability and Protection against Machine Errors

In order to allow the program to operate within the normal operating system and schedule, we have provided for the breaking up of the longer runs into sections. This is accomplished by specifying in the input data where in the sequence of the calculations to begin and where to end. This permits the calculation of the matrices and various contributions to the supermatrices to be made independently as time is available. Thus, a run which may take 5 hr in total can be divided into as many as 7 shorter runs much easier to schedule. We have found this feature essential, particularly in an environment where the computer is near saturation and long runs difficult to process. This same feature affords protection against machine error in that the useful results accumulated prior to the point of failure have been saved and the calculation can be recommenced at or near this point (see JFLG and KFLG in input specifications, Sect. IV).

C. Prescreening of Input Decks

With a program of this sort, it is often necessary to leave large amounts of input data at the computation site to be run at night when time and scheduling permits. It is, therefore, crucial that the submitted input decks be free of errors since the user will not usually be available to make corrections. We have, therefore, provided for preprocessing of the prepared input decks to detect errors and insure that they will be valid runs when submitted (see JFLG). The prescreening of input which involves only seconds of computer time during the normal schedule has already saved us much disappointment and many lost evenings and weekends of potentially fruitful calculations.

D. Performing the SCF Procedure Using Previously Computed Integrals

Frequently, a SCF run, particularly for a molecular system new to the user or because of unscreenable input errors, will fail to converge.

It is often possible with minor changes in the input effecting the SCF process to achieve convergence. We, therefore, have provided for the saving of the matrices and supermatrices, and the running of the inexpensive SCF process from previously computed integrals (see KFLG in input specifications, Sect. IV).

E. Handling of Tape and Disk Errors

Normal operating system procedures.

F. Subroutine Structure

A detailed presentation of the code and subroutine structure is given in Part 2 (in preparation) of this report series.¹¹

G. Use as an Atomic SCF Program

The program can be used without modification to calculate SCF solutions for atoms. In this case only the one-center integrals are computed; however, there are inefficiencies due to the overall diatomic design of the program. The SCF solution obtained will be that for an atom with $C_{\infty v}$ symmetry (i.e., a preferred axis), however, the wavefunction and energy thus obtained is very close to the spherically symmetrical solution. We have found it quite useful to do pilot atomic SCF calculations with the program, particularly during basis set exploration, thus avoiding the often time-consuming task of familiarization with another program written specifically for the atomic case.

IV. INPUT AND OUTPUT*

The input to the program has been kept to the essential minimum. When possible, data are provided internally by the program. Input is thoroughly screened by the program to prevent costly erroneous calculations. In the following, the input symbol, its description, and when possible, the suggested value are given. The FORTRAN format for the input cards is then tabulated, limitations listed, and sample input and output given (see Tables 1, 2, and 3).

TABLE 1. Description of Input Variables for CDC-3600*

Symbol	Description
Title	10-word title of run; for example, "LiCl NOMINAL BASIS SET R = 4.0 bohrs."
R	Internuclear distance

*See Appendix E for IBM 360/75 input specifications.

TABLE 1 (Contd.)

Symbol	Description
RMAX	This truncates the upper limit in the numerical integrations. If omitted RMAX = 60.0 Bohrs is assumed. RMAX may be computed by the following equation: $RMAX \approx 60.0/2\zeta_{min}$, where ζ_{min} is the smallest orbital exponent in the basis set.
NP1 NP2	Specifies the number of gauss points on xi, and eta, respectively; used in the gaussian numerical integration section of the Coulomb-hybrid programs. If omitted, NP1 = NP2 = 30 is substituted. The allowed grid sizes are 12, 16, 20, 24, 30, 36, 40, 50, 60, 70, 80, 90, and 100. If the requested grid is different than those in stock, the program will substitute the grid size nearest to the requested size. See Sect. V-B for grid specifications.
NFHD	Homopolar or heteropolar flag = 1 Homo = 0 Heter
ZA	Nuclear charge on center A
ZB	Nuclear charge on center B
NP4	Specifies the number of Simpson-rule points used in the numerical integration section of the exchange programs. NP4 is restricted to the range $0 \leq NSIMP \leq 94$. See Sect. V-B for the grid specifications. (Suggested value, 50.)
NP3	Number of Neumann iterations employed. (Suggested value, 10.) Maximum permitted, 40.
NOEL	Bias for one-electron matrix integration. (Suggested value, 20.)
LFLAG	OPEN SHELL FLAG. If $\neq 0$, signifies open-shell calculations. If = 0, signifies closed shells only.
IFLAG	SCF printing flag. If < 0 , suppresses all printout except for final two iterations; if = 0 or positive, prints all iterations and extrapolations.
ITFL	Integrals print flag. If $\neq 0$, then S, U, J, K, P, Q, T, H, F, and supermatrices will be printed. If = 0, only S, H, and F are printed.
IPUNCH	If $\neq 0$, output deck is punched.

TABLE 1 (Contd.)

Symbol	Description
KFLG } JFLG }	<p>Calculation option flag. Specifies at what stage of diatomic calculation is to be started (KFLG) ended (JFLG)</p> <p>= 0. Do entire calculation. = 1. Start with screening. End = 2. Start with J exchange integrals. End = 3. Start with J Coulomb-hybrid integrals. End = 4. Start with K exchange integrals. End = 5. Start with K Coulomb-hybrid integrals. End = 6. Start with S, U, and T. End = 7. Start with construction P and Q. (= 11 for homo-nuclear calculation) End = 8. Start with SCF procedure. End = 9. Start with calculation of molecular properties. End = 10. Start with plotting of orbital and total charge density contours. End</p>
CFLG	≠ 0 Crystal field matrix present.
IPRCT	Prior SCF iterations before extrapolations are begun. (Suggested value, 5.)
EPS	SCF convergence threshold. SCF process is terminated when the differences between all vector components from two successive iterations is less than this number. Suggested value 0.001 (very loose); 0.0000001 (tight). A value of 0.00001 yields usual desired accuracy in vectors.
CHCONV	Convergence threshold for calculation of electrostatic potentials in integral computation. A value of 0.0000001 suggested.
NLAMDA	Number of basis functions in current symmetry block.
NORBS	Number of occupied orbitals in current symmetry block.
SIGL	Inversion symmetry parameter u or g for homonuclear case. $\sigma_g + 1.0$, $\sigma_u - 1.0$, $\pi_u + 1.0$, $\pi_g - 1.0$, etc.

TABLE 1 (Contd.)

Symbol	Description
NC	Number of closed-shell orbitals in current symmetry block.
NO	Number of open-shell orbitals in current symmetry block.
CM	Closed-shell occupation numbers. NLAMDA of these must be given (blank indicates zero). Nonzero value of n^{th} CM indicates n^{th} orbital occupation in current symmetry.
CM	Open-shell occupation numbers. Not necessary if closed-shell case. If LFLAG $\neq 0$, the NLAMDA CM's must be given.
N, L, M, ZETA	The quantum numbers n , l , m of the basis function and the orbital exponent ζ . ζ is + if on center <u>a</u> ; - if on center <u>b</u> .
CIP	Vector Components. NLAMDA of these are given for each occupied orbital, first for the closed shells and then the open. A blank card would now follow if the current symmetry block is the last one. If not, card pattern is repeated from NLAMDA.
A B C	The $A_{\lambda\mu}$, $B_{\lambda\mu}$, $C_{\lambda\mu}$ vector-coupling coefficients for the open-shell cases. Needed only if open shells are present. Given as a matrix on symmetries λ and μ (see Table 3a).
CRYSTAL	Crystal field matrix if CFLAG $\neq 0$

TABLE 2: Input Cards and Their Format¹¹

Card No.	Format	Contents
1	10A8	Title
2	2F10.4, 4I5, 2F5.1	R, RMAX, NP2, NP1, NFHD, NFC/EF, ZA, ZB
3	3I5	NP3, NP4, N/EL
4	5I5, 2E12.9, 3I5	LFLAG, IFLAG, ITFL, KFLG, IPRCT, EPS, CHCONV, IPUNCH, JFLG, CFLG
5	4I5 15, F5.1, 3I5	NLAMDA, NORBS, NC, NO (if hetero) NLAMDA, SIGL, NORBS, NC, NO (if homo)

TABLE 2 (Contd.)

Card No.	Format	Contents
6	16F5.1	CM(closed shell)
6 +]NLAMDA/16[	16F5.1	CM(open shell)
6 + NLAMDA/16 + NLAMDA/16		
next	3I5, F10.5	N (1) , L (1) , M (1) ZETA (1)
+NLAMDA-1		N(NLAMDA), L(NLAMDA), M(NLAMDA), ZETA(NLAMDA)
Next +NLAMDA	F10.5	CIP
		. closed
		. open
Next +NORBS x NLAMDA		blank if last symmetry block repeat from card 5 if not.
	3F12.8	
(one card for each λ , μ symmetry block)		A(1,1), B(1,1), C(1,1) A(1,2), B(1,2), C(1,2)
		A(λ , λ), B(λ , λ), C(λ , λ) where λ is highest symmetry present.

TABLE 2 (Contd.)

Card No.	Format	Contents
	5F16.8	Crystal field matrix if CFLG $\neq$ 0.
New Data Deck or If Last Case		
Last	10A8	"End of Run"

TABLE 3. Program Limitations

1. MATRIX SIZE LIMITED TO 1000 ELEMENTS.
2. NUMBER OF SUPERMATRIX ELEMENTS LIMITED TO 1,500,000.
3. QUANTUM NUMBERS $1 \leq N \leq 8$; $0 \leq L \leq N-1$; $-L \leq M \leq L$.
4. VECTORS LIMITED TO A TOTAL OF 500 COMPONENTS.
5. NUMBER OF BLOCKS LIMITED TO 4.
6. NUMBER OF BASIS FUNCTIONS LIMITED TO 100.
7. NUMBER OF GAUSS POINTS LIMITED TO 100 ON EACH COORDINATE.
8. SIMPSON'S POINTS LIMITED TO 94.
9. NEUMANN ITERATIONS LIMITED TO 40.
10. NUMBER OF ORBITALS/BLOCK LIMITED TO 20.

TABLE 3a. Open-shell Vector-coupling Coefficients

Single Open Shells

Configuration	States	$A_{\lambda\lambda}$	$B_{\lambda\lambda}$	$C_{\lambda\lambda}$
σ	$^2\Sigma^+$	1	$-1/4$	$-1/4$
π	$^2\Pi$	1	$-1/4$	$-1/4$
δ	$^2\Delta$	1	$-1/4$	$-1/4$
$\pi^2; \delta^2, \sigma\sigma^1$	$^3\Sigma; ^3\Sigma$	0	$1/4$	$1/4$
$\pi^2\delta^2$	$^1\Delta; ^1\Gamma$	$1/2$	$-1/4$	$-1/4$
$\pi^2\delta^2$	$^1\Sigma; ^1\Sigma$	1	$-3/4$	$-3/4$
$\pi^3; \delta^3$	$^2\Pi; ^2\Delta$	$1/9$	$-1/36$	$-1/36$

Off-diagonal Elements for Double Open Shells*

Configuration	States	$A_{\sigma\mu}$	$B_{\sigma\mu}$	$C_{\sigma\mu}$
$\sigma\pi$	$^3\Pi$	0	$1/4$	$1/4$
	$^1\Pi$	0	$-3/4$	$-3/4$
$\sigma\pi^2$	$^4\Sigma^-(\pi^2, ^3\Sigma^-)$	0	$1/4$	$1/4$
	$^2\Sigma^-(\pi^2, ^3\Sigma^-)$	0	$-1/2$	$-1/2$
	$^2\Delta(\pi^2, ^1\Delta)$	0	0	0
	$^2\Sigma^+(\pi^2, ^1\Sigma^+)$	0	0	0
$\sigma\pi^3$	$^3\Pi$	0	$1/12$	$1/12$
	$^1\Pi$	0	$-1/4$	$-1/4$
$\sigma\delta$	$^3\Delta$	0	$1/4$	$1/4$
	$^1\Delta$	0	$-3/4$	$-3/4$
$\sigma\delta^2$	$^4\Sigma^-(\delta^2, ^3\Sigma^+)$	0	$1/4$	$1/4$
	$^2\Sigma^-(\delta^2, ^3\Sigma^+)$	0	$-1/2$	$-1/2$
	$^2\Gamma(\delta^2, ^1\Gamma)$	0	0	0
	$^2\Sigma^-(\delta^2, ^1\Sigma^+)$	0	0	0
$\sigma\delta^3$	$^3\Delta$	0	$1/12$	$1/12$
	$^1\Delta$	0	$-1/4$	$-1/4$

*Diagonal coefficients are the same as those given for single open shells.

[illegible]

A. Sample Input for NaCl

HETERONUCLEAR DIATOMIC NaCl DATA - IONIC BASIS

4.461 20.00 36 36 0 1 11.0 17.0
 10 36 30
 1 10 .00001 .0000001 1
 17 8 8 0
 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0

1 0 0 15.314
 1 0 0 10.157
 3 0 0 6.254
 2 0 0 2.966
 2 1 0 8.000
 2 1 0 4.316
 2 1 0 2.325
 1 0 0 -18.542
 2 0 0 -16.300
 2 0 0 -6.084
 3 0 0 -2.606
 3 0 0 -1.4860
 2 1 0 -10.206
 2 1 0 -5.586
 3 1 0 -2.496
 3 1 0 -1.223
 3 2 0 -2.5

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.85416

0.17380

0.00167

-0.00019

0.00006

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.09647

0.90707

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00573

-0.00031

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

0.00000

-0.23890

-0.14234

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B. Sample Output for NaCl

By A. C. Wahl, P. J. Bertoncini, and K. Kaiser, Chemistry Division,
and R. H. Land, Solid State Science Division,
Argonne National Laboratory
June 18, 1968

HETERONUCLEAR DIATOMIC NaCl DATA - IONIC BASIS
ZA = 11.000 ZB = 17.000

INTERNUCLEAR DISTANCE = 4.4610 BOHRS
INTEGRATION TRUNCATED AT 20.0000 BOHRS
NUMBER OF NEUMANN ITERATIONS = 10
BIAS FOR ONE ELECTRON GRID = 30
VECTOR COEFFICIENT DIAGONALIZATION THRESHOLD = 1.000E-05
PRIOR ITERATIONS = 10
COULOMB-HYBRID CONVERGENCE THRESHOLD = 1.000E-07

BASIS SET BLOCK I					ORBITAL COEFFICIENTS							
N	L	M	ZETA	CENTER	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)
1	0	0	15.31400	A	=0.00000	0.09647	=0.00000	=0.00000	=0.00001	=0.00000	=0.00000	=0.00000
1	0	0	10.15700	A	=0.00000	0.90707	=0.00000	=0.00000	=0.26474	=0.00000	=0.00000	=0.00000
3	0	0	6.25400	A	=0.00000	0.00573	=0.00000	=0.00000	0.26942	=0.00000	=0.00000	=0.00000
2	0	0	2.96600	A	=0.00000	=0.00031	=0.00000	=0.00000	0.79097	=0.00000	=0.00000	=0.00000
2	1	0	8.00000	A	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	0.06123	=0.00000	=0.00000
2	1	0	4.31600	A	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	0.45069	=0.00000	=0.00000
2	1	0	2.32500	A	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	0.56481	=0.00000	=0.00000
1	0	0	18.54200	B	0.85416	=0.00000	=0.23890	=0.00000	=0.00000	=0.00000	0.07030	=0.00000
2	0	0	16.30000	B	0.17350	=0.00000	=0.14234	=0.00000	=0.00000	=0.00000	0.05232	=0.00000
2	0	0	6.08400	B	0.00167	=0.00000	1.08092	=0.00000	=0.00000	=0.00000	=0.38891	=0.00000
3	0	0	2.60600	B	=0.00019	=0.00000	0.01891	=0.00000	=0.00000	=0.00000	0.81927	=0.00000
3	0	0	1.48600	B	0.00006	=0.00000	=0.00581	=0.00000	=0.00000	=0.00000	0.29108	=0.00000
2	1	0	10.20600	B	=0.00000	=0.00000	=0.00000	0.21098	=0.00000	=0.00000	=0.00000	=0.05024
2	1	0	5.58600	B	=0.00000	=0.00000	=0.00000	0.81807	=0.00000	=0.00000	=0.00000	=0.21345
3	1	0	2.49600	B	=0.00000	=0.00000	=0.00000	0.01592	=0.00000	=0.00000	=0.00000	0.61093
3	1	0	1.22300	B	=0.00000	=0.00000	=0.00000	=0.00396	=0.00000	=0.00000	=0.00000	0.52375
3	2	0	2.50000	B	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000	=0.00000

NUMBER OF ELECTRONS OCCUPYING
CLOSED SHELL ORBITALS = 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0

BASIS SET BLOCK II					ORBITAL COEFFICIENTS		
N	L	M	ZETA	CENTER	C(1)	C(2)	C(3)
2	1	1	8.00000	A	=0.00000	0.06123	=0.00000
2	1	1	4.31600	A	=0.00000	0.45069	=0.00000
2	1	1	2.32500	A	=0.00000	0.56481	=0.00000
2	1	1	10.20600	B	0.21098	=0.00000	=0.05024
2	1	1	5.58600	B	0.81807	=0.00000	=0.21345
3	1	1	2.49600	B	0.01592	=0.00000	0.61093
3	1	1	1.22300	B	=0.00396	=0.00000	0.52375
3	2	1	2.50000	B	=0.00000	=0.00000	=0.00000

NUMBER OF ELECTRONS OCCUPYING
CLOSED SHELL ORBITALS = 4.0 4.0 4.0

H=MATRIX

-5,50055064+001	-6,21047352+001	-6,39554793+001	-1,55487332+001	-1,98136666+001	-2,28308863+001
-1,06792129+001	-1,35375388+001	-1,92195948+001	-1,86576120+001	-4,30534506+002	-8,11684004+002
-1,60134447+001	-1,24453545+001	-1,58197808+001	-2,17505364+002	-5,39254298+002	-2,77648756+001
-3,10292492+001	-1,61628811+001	-1,82657163+001	-7,90779974+003	-2,40723989+002	-2,54869439+001
-4,49161259+001	-9,32851264+000	-1,35191884+001	-1,40017607+001	-1,89051451+026	-2,19597163+017
-3,83235500+008	-1,16627413+003	-5,97387443+012	-1,31915855+005	-1,88388689+002	-1,45776930+002
-1,07797764+024	-6,66277323+017	-6,00036418+008	-1,51651103+003	-1,16850306+011	-1,82404278+005
-2,39996767+002	-1,25992660+002	-9,67341468+001	-9,33532869+009	-1,14904222+008	-2,35439328+006
-3,85864807+003	-8,70519300+008	-9,51125329+005	-9,00926024+002	-4,44142534+001	-5,00632950+001
-4,80106384+001	-1,30592051+002	-1,69214695+002	-4,51126661+002	-1,34997891+001	-1,28147058+002
-5,23646387+002	-3,85804693+001	-1,81406133+000	-3,69320185+000	-1,17300677+001	-1,65540216+001
-2,62007290+001	-3,30330835+001	-6,43957541+001	-1,04296906+000	-1,09901718+001	-3,28572943+001
-1,09758693+000	-3,34266309+001	-7,57310503+001	-4,53240118+000	-1,05062694+001	-1,06602241+001
-9,53060041+016	-1,83656882+014	-1,4826094+007	-1,02739350+003	-9,44994056+011	-2,18201389+005
-1,18063300+002	-2,39337268+002	-5,25570329+002	-8,30181976+002	-1,87689180+002	-4,98530209+003
-3,71391650+001	-7,68683372+008	-1,28608613+007	-9,82666554+006	-3,89221298+003	-6,46949797+007
-1,72199892+004	-3,66994162+002	-1,27368353+002	-3,67545760+002	-1,36109357+001	-9,52009844+002
-3,73018745+002	-3,28481973+001	-3,43570293+001	-4,16049233+002	-4,07591270+002	-1,02727567+001
-2,64035011+001	-2,87428718+002	-1,09770180+001	-6,18647594+001	-7,30608677+004	-3,55693519+003
-7,33037719+002	-4,37130432+001	-4,44224612+001	-2,21902620+000	-1,04527193+001	-1,52675019+001
-7,38412316+001	-9,27232893+001	-1,72539036+000	-2,55922584+000	-2,28356235+001	-6,51630021+001
-1,85163954+000	-8,74919899+005	-4,78532318+004	-1,85780500+002	-3,57304715+001	-7,77265521+001
-8,25242214+001	-2,27837409+000	-8,14465139+000	-9,43021896+000	-4,02275369+002	-5,17873976+002
-1,27390434+001	-2,95902372+001	-3,62277945+002	-1,32891677+001	-5,98708505+001	-3,63305491+005
-2,30902959+004	-1,04030492+002	-1,18835704+001	-1,54158885+001	-1,55582172+002	-8,28919096+002
-4,37175225+001	-4,03120093+001	-1,36010954+001	-1,58063165+001	-1,61449042+001	-1,82194566+001
-9,31535661+000	-1,34574293+001	-1,38420551+001	-2,76753734+012	-1,20126590+006	-1,26137126+003
-3,71338123+001	-2,74605561+008	-9,82120070+006	-3,96325140+003	-3,28410469+001	-3,43391602+001
-3,15181438+003	-1,24390766+002	-8,7393214+002	-5,21682531+000	-1,04345624+001	-1,51004561+001
-6,45091387+002	-1,85250430+001	-5,73402693+001	-8,24820375+001	-2,27248344+000	-7,95105306+000
-8,81715702+000	-6,88532430+003	-2,62977602+002	-1,50952072+001	-1,32249606+002	-6,85653471+002
-3,24836225+001	-2,66380768+001	-1,35375686+001			

S=MATRIX

9,99999983+001	9,39146048+001	9,99999986+001	1,58970349+001	3,36670831+001	9,99999993+001
1,12669580+001	2,29130429+001	8,81422754+001	9,99999994+001	1,79707099+009	1,96224411+009
1,18916150+009	8,54871544+010	9,99999986+001	6,24159729+010	8,59618121+010	1,27688526+009
1,26295863+009	7,91097114+001	9,99999990+001	1,81928619+010	2,84950308+010	1,03490666+009
1,12582168+009	4,06894700+001	7,90211883+001	9,99999993+001	1,11303501+028	1,33686543+019
2,37446900+010	7,27334133+006	3,67644990+014	8,20818511+008	1,17578204+004	9,99999981+001
8,44763226+027	6,42919487+019	6,21394840+010	4,59433864+005	1,18332018+013	1,90904802+007
2,52661003+004	8,05271221+001	9,99999987+001	6,84310081+011	1,95784357+010	8,74166510+008
1,15915869+004	2,72714889+009	3,22050791+006	1,43256059+003	2,74652140+001	5,57703683+001
9,99999992+001	1,47448150+004	2,83900900+004	2,15561273+003	9,22900503+003	4,75904628+004
3,13240340+003	2,84253302+002	1,09138697+002	3,92076558+002	3,53878471+001	9,99999995+001
2,97315822+003	5,53429979+003	3,04650568+002	6,93194618+002	4,10298188+003	1,94028271+002
8,76651345+002	2,00584368+003	7,91871046+003	1,13384299+001	7,61442065+001	9,99999997+001
9,38069959+018	3,07449633+016	3,04200782+009	2,20224781+005	1,84513465+012	4,60818052+007
2,54200948+004	2,41014782+009	2,56584277+009	1,54204079+009	1,81565629+010	4,34049032+011
9,99999984+001	8,37332673+010	2,18493687+009	3,61254518+007	1,52831742+004	2,09920152+008
7,10192879+006	1,40724591+003	8,76838849+010	1,16065294+009	1,53449492+009	5,17173537+010
1,58772511+010	7,99568239+001	9,99999989+001	3,57125992+004	6,83645063+004	4,90001335+003
1,80218223+002	1,07037947+003	6,56670817+003	4,71066400+002	2,12862848+011	5,98940236+011
4,47320442+010	1,09889714+009	6,71581943+010	1,13723872+001	3,79825950+001	9,99999994+001
8,38572174+003	1,55324599+002	8,14900763+002	1,67915669+001	8,46799747+003	3,78902875+002
1,45746487+001	2,22181572+012	6,99028028+012	8,68716434+011	5,30114166+010	9,78024125+010
1,76470233+002	8,74649939+002	6,46510156+001	9,99999995+001	4,54696178+004	8,68503345+004
6,06810628+003	2,00261006+002	1,35114365+003	7,94222452+003	4,60337352+002	-6,62746598+011
-1,78225720+010	-9,75739969+010	-1,97910147+009	-1,29800271+009	3,49632672+010	8,34411481+010
1,56275815+009	9,53647798+010	9,99999993+001	9,99999993+001	7,91097718+001	9,99999995+001
4,06894702+001	7,90211886+001	9,99999995+001	5,41276662+014	2,54412952+008	2,73111700+005
9,99999993+001	8,96535823+010	4,10904592+007	1,54330499+004	7,99568244+001	9,99999994+001
1,19164822+004	7,73508923+004	7,23078487+003	1,13723873+001	3,79825951+001	9,99999996+001
2,49280477+003	1,16554258+002	5,24503692+002	1,76470234+002	8,74649943+002	6,46510158+001
9,99999997+001	2,60640515+004	1,63404512+003	1,26604854+002	1,44664222+011	1,45371740+010
3,33984750+010	1,83757939+010	9,99999996+001			

U MATRIX

1.722648003+002	1.351443407+002	1.155378025+002	1.003465431+001	1.647702554+001	2.674213789+001	7.981228126+000
1.189870448+001	2.123770915+001	2.012380461+001	4.305374208+002	8.116864520+002	1.601344683+001	1.244535606+001
4.781978019+001	2.175058608+002	5.392547586+002	2.776487697+001	3.102925009+001	2.982039196+001	2.757964418+001
7.907807182+003	2.407240652+002	2.548694440+001	4.491612630+001	1.311263333+001	1.748395803+001	1.670457315+001
6.290767301+027	1.538020994+017	3.465857287+008	1.143653247+003	4.932590374+012	1.258770769+005	1.864431954+002
3.176798053+002	1.482778721+025	3.507148614+017	5.046307382+008	1.467095121+003	8.347418925+012	1.684095116+005
2.358333461+002	1.609767884+002	1.410158128+002	5.256882054+009	8.432950736+009	1.322191511+006	3.518281467+003
4.661461727+008	7.347973136+005	4.746544345+002	3.900421492+001	5.443066070+001	5.417981435+001	1.279679805+002
1.642025066+002	4.168521365+002	1.251943366+001	1.207327594+002	4.830094308+002	3.696970696+001	1.007839278+000
2.616962613+000	1.132829210+001	1.723314519+001	2.612554545+001	3.289501031+001	6.373823735+001	1.032928111+000
1.095529160+001	3.278194095+001	1.103278324+000	1.756796954+001	4.983894994+001	3.197869762+000	1.070562377+001
1.088104368+001	5.104492789+016	5.104742930+015	1.030930695+007	9.621515701+004	4.428796206+011	1.853471833+005
1.142193810+002	2.393453674+002	5.255737885+002	8.301828467+002	1.876891908+002	4.985301989+003	8.922038180+001
6.595153603+008	1.003651532+007	5.077648201+006	3.468383428+003	3.878979463+007	1.272685337+004	3.472341937+002
1.273694583+002	3.675465696+002	1.361093931+001	9.520098653+002	3.730187473+002	5.564017613+001	4.995872703+001
3.106022120+002	3.972709730+002	9.615398918+002	2.485730700+001	2.736013132+002	1.029178879+001	6.017871578+001
7.306062809+004	3.556933544+003	7.330377244+002	4.371304344+001	4.442246130+001	5.193259419+000	1.138584641+001
1.672117225+001	7.382098024+001	9.268953949+001	1.725387028+000	2.566479109+000	2.297881245+001	6.593394399+001
1.892533086+000	8.749142291+005	4.785320785+004	1.857804986+002	3.573047157+001	7.772655212+001	7.295341411+001
2.244466675+000	8.535298641+000	9.779222392+000	3.95771821+002	5.056078047+002	1.199980843+001	2.821643187+001
3.465708882+002	1.259526579+001	5.927364673+001	3.632734379+005	2.308974106+004	1.040383803+002	1.188356969+001
1.541588811+001	1.555822431+002	8.289191898+002	4.371752310+001	4.031200945+001	1.672609539+001	4.780631630+001
2.980241525+001	2.753338473+001	1.309947733+001	1.742219896+001	1.654516764+001	1.285658525+012	1.016808710+006
1.216846311+003	8.921502984+001	1.625619273+008	7.142506481+006	3.725176478+003	5.563302592+001	4.994085811+001
2.976846015+003	1.146600334+002	8.306324793+002	5.191058930+000	1.136768949+001	1.655412645+001	6.446848152+002
1.853251132+001	5.767677429+001	7.291123015+001	2.238576022+000	8.341700314+000	9.166160452+000	6.529615287+003
2.445942205+002	1.455355121+001	1.322496023+002	6.856534803+002	3.248362271+001	2.663807682+001	1.666256854+001

T MATRIX

1.172592939+002	7.303940548+001	5.158232315+001	-5.514078867+000	-3.336641110+000	3.911251570+000	-2.697984742+000
-1.638834310+000	2.018114358+000	1.466192656+000	2.914674138+007	2.447848015+007	2.082899334+008	1.591845182+008
3.199999938+001	4.971843848+008	4.606243324+008	1.413183191+008	9.308604312+009	1.365751089+001	9.313927880+000
7.444628634+009	7.667188021+009	5.247640223+009	4.436734954+009	3.784120697+000	3.964769588+000	2.702812475+000
-1.261413778+026	-6.579506409+018	-3.664977086+009	-2.262057924+005	-1.041284060+012	-6.038778109+007	-1.945493264+004
1.719028750+002	-9.296997720+025	-3.155624620+017	-9.540567944+009	-4.941590508+005	-3.337611678+012	-1.399476596+006
-4.163421227+004	3.498412836+001	4.428166603+001	-1.078446638+009	-3.057471508+009	-1.032201771+006	-3.403666023+004
-4.043731271+008	-2.163280154+005	-2.227158918+003	-5.410038499+000	4.367365677+000	6.169175942+000	-2.627070832+004
-5.012188370+004	-3.427452422+003	-9.803554256+003	-7.414298416+004	-4.063695650+003	-1.610562337+002	-8.062220468+001
-1.076239240+000	-4.017755670+001	6.791235975+001	-7.513807321+003	-1.380732176+003	-6.575167854+003	-1.004094639+002
-3.488024911+004	-7.535337047+004	5.691390309+003	-1.585866134+001	-2.589210034+001	-3.345314147+001	1.993543665+001
2.208195997+001	-4.426107620+016	-1.326094523+014	-4.517202426+008	-6.524193455+005	-5.021144355+011	-3.285420532+006
-3.843918876+004	4.099344444+007	3.459567417+007	8.705169524+008	1.081441333+009	-1.000454896+010	5.208121683+001
-1.091680114+008	-2.843459971+008	-3.749017336+006	-4.238296544+004	-2.590518509+007	-4.493135798+005	-1.976196846+003
1.105453065+007	8.099347912+008	3.767558311+008	2.133586391+009	2.696824650+010	2.279197879+001	1.560169776+001
-5.447020731+004	-1.032029659+003	-6.573577547+003	-1.546194067+002	-1.382740522+003	-6.852292398+003	-1.686043587+002
-2.396571901+009	-1.642405807+009	5.592748608+010	2.151446988+009	9.598768646+010	-2.576677804+002	9.331270729+001
1.453670390+000	-2.025136333+004	-3.404979728+004	-3.328661023+006	7.253268177+003	1.431889453+003	7.709419025+003
4.089354832+002	-2.669777994+010	-2.396349247+010	-1.784210651+010	4.331673551+010	4.450416295+010	-9.570807285+002
-3.390741395+002	3.906472531+001	3.490034311+001	-6.503506907+004	-1.226617105+003	-7.392349457+003	-1.373805287+002
-1.570705729+003	-6.939018621+003	-5.972037477+003	-3.205350406+009	-5.548650589+009	-1.117563504+008	-7.588246256+009
-3.489942864+009	7.119388944+009	9.381458251+009	5.95461044+009	1.708590603+009	3.124999970+000	3.199999976+001
1.365751100+001	9.313927941+000	3.784120723+000	3.964769608+000	2.702812488+000	-1.481878816+012	-1.864071854+007
-4.452494645+005	5.208121759+001	-1.120416338+008	-2.78694220+006	-2.380749202+004	2.279197903+001	1.560169789+001
-1.749683618+004	-9.730732818+004	-4.330073448+003	-2.576678895+002	9.331270756+001	1.453670391+000	-4.065716642+005
7.168336594+005	3.365049461+003	-9.570807369+002	-3.390741412+002	3.906472545+001	3.490034322+001	-3.557390159+004
-1.838338153+003	-5.416560231+003	-3.677151143+010	9.406193450+010	1.820400834+009	3.283232773+010	3.124999982+000

S MATRIX

9.999999827+001	9.391460484+001	9.999999861+001	1.589703493+001	3.366708306+001	9.999999933+001	1.126695799+001
2.291364289+001	8.814227542+001	9.999999940+001	1.797070992+009	1.962244110+009	1.189161505+009	8.548715438+010
9.999999862+001	6.241597291+010	8.596181206+010	1.276885256+009	1.262958633+009	7.910977139+001	9.999999902+001
1.819286191+010	2.849503080+010	1.034906658+009	1.125821684+009	4.068946996+001	7.902118831+001	9.999999929+001
1.113053008+028	1.336865427+019	2.374469001+010	7.273321330+006	3.676449899+014	8.208185114+008	1.175782038+004
9.999999980+001	8.447632251+027	6.429194870+019	6.213948401+010	1.594338860+005	1.183320176+013	1.909048018+007
2.526610033+004	8.052712207+001	9.9999999873+001	6.843100814+011	1.957843569+010	8.741665103+008	1.159158693+004
2.727148892+009	3.220507909+006	1.432560593+003	2.746521498+001	5.577036829+001	9.999999921+001	1.474451499+004
2.839008996+004	2.155612720+003	9.229005029+003	4.759046279+004	3.132403400+003	2.842533022+002	1.091386974+002
3.920765578+002	3.538784714+001	9.999999954+001	2.973158216+003	5.534259786+003	3.046565684+002	6.931946179+002
4.102981884+003	1.940282717+002	8.766513446+002	2.005823680+003	7.918710455+003	1.133842986+001	7.614420649+001
9.999999966+001	9.380699588+018	3.074456332+016	3.042007815+009	2.202247807+005	1.845134647+012	4.608180518+007
2.542009479+004	2.410197819+009	2.565842769+009	1.542040791+009	1.815656294+010	4.340490321+011	9.999999839+001
8.373326732+010	2.184936867+009	3.612545182+007	1.528317417+004	2.099201515+008	7.101928794+006	1.407215905+003
8.768388494+010	1.160652942+009	1.534494917+009	5.171735467+010	1.587725109+010	7.995682386+001	9.999999889+001
3.571259917+004	6.836450634+004	4.900013349+003	1.802182233+002	1.070379446+003	6.566708166+003	4.710664002+002
2.128628478+011	5.989402362+011	4.473204421+010	1.098897141+009	6.715819431+010	1.137238724+001	3.798259498+001
9.999999937+001	8.385721744+003	1.553205992+002	8.149007632+002	1.679156687+001	8.467997471+003	3.789028748+002
1.457464870+001	2.221815722+012	6.990280278+012	8.687164338+011	5.301141662+010	9.780241254+010	1.764702333+002
8.746499395+002	6.465101564+001	9.999999953+001	4.546961779+004	8.685033452+004	6.068106285+003	2.002610061+002
1.351193650+003	7.942224519+003	4.603373524+002	-6.627465983+011	-1.782257201+010	-9.757399686+010	-1.979101475+009
-1.298002708+009	3.496326717+010	8.344114807+010	1.562758147+009	9.536477796+010	9.999999931+001	9.999999933+001
7.910977185+001	9.999999949+001	4.068947017+001	7.92118865+001	9.999999953+001	5.412766619+014	2.544129524+008
2.731117001+005	9.999999938+001	8.965358234+010	4.109045919+007	1.543304994+004	7.995682440+001	9.999999943+001
1.191648215+004	7.735089227+004	7.230784870+003	1.137238730+001	3.798259513+001	9.999999962+001	2.492804774+003
1.165542580+002	5.245036921+002	1.764702342+002	8.746499427+002	6.465101580+001	9.999999972+001	2.606485147+004
1.634045120+003	1.266048541+002	1.446642225+011	1.453717398+010	3.339847498+010	1.837579390+010	9.999999957+001

P-MATRIX

2,55247896+001	2,29069177+001	2,35470618+001	3,02496656+000	6,60876841+000	1,67375812+001
2,24441816+000	4,48401013+000	1,37179351+001	3,40177234+001	4,94197390+002	8,86596462+002
1,64247068+001	1,28850576+001	2,22692435+001	2,55402689+002	5,82608219+002	2,87794923+001
3,24512185+001	1,56807755+001	1,70965906+001	9,32967009+003	2,58674100+002	2,87193246+001
4,70205880+001	7,21421831+000	1,18745810+001	1,29100779+001	-3,90174705+006	6,90179954+007
2,59812816+005	2,50180308+004	4,06446959+005	4,73146440+005	4,15662361+003	4,30394113+001
3,24722107+005	-8,82454159+006	-2,18852686+004	6,52002048+004	-2,94441953+004	-2,87099503+004
8,88308475+003	3,21069651+001	3,88351342+001	-6,68057849+006	3,26806152+006	3,28465671+005
2,20178618+003	2,57617756+005	5,64364718+005	2,94087404+002	9,91248183+000	1,91393527+001
2,72972634+001	2,78593936+003	5,49532168+003	5,06832710+002	1,04384516+001	8,43297167+003
3,97451912+002	3,22694825+001	3,28791386+001	1,04293977+000	7,33573034+000	1,41921897+001
6,40290289+002	1,08147600+001	4,22397487+001	8,19325036+001	5,63278693+002	2,49326362+001
9,88919222+001	5,53656718+002	2,14583560+001	4,16837900+000	9,18134893+000	9,89385575+000
2,06272800+004	-4,03484726+005	-1,19934927+003	1,17055379+003	-1,32100119+003	-1,19993032+003
8,93243824+003	2,12347745+002	5,02715618+002	8,05852446+002	1,56610957+002	4,12390470+003
3,53656656+001	-4,73472843+005	1,11814454+005	2,70046437+004	2,37578080+003	3,06823960+004
3,67191472+004	2,43302189+002	1,16393686+002	3,53685893+002	1,31465595+001	9,03224011+002
3,47342043+002	2,49903942+001	2,68575698+001	6,72624033+003	1,32274672+002	7,63361708+002
2,06094358+001	1,81898455+002	8,35612573+002	9,32419981+001	1,11623319+003	1,94214658+003
6,96443379+002	4,15540576+001	4,09799271+001	2,74867170+000	7,74831561+000	1,41230783+001
1,80162975+001	3,04560117+001	1,13967639+000	2,00485548+000	1,21922650+001	5,03809379+001
1,69550635+000	3,57244568+004	-6,42639411+004	1,72843608+002	3,33371748+001	6,93468263+001
4,28419567+001	1,60339481+000	7,51641049+000	9,12288532+000	9,96783470+003	1,65820833+002
7,99023983+002	2,36114109+001	1,40754954+002	9,37418770+002	5,39769446+001	-4,77681757+005
5,01488662+004	9,74350741+003	1,05146137+001	1,35116677+001	1,72982052+002	7,95512278+002
4,01340423+001	3,60716439+001	1,46687325+001	2,22610066+001	1,56676142+001	1,70542283+001
7,20222491+000	1,18144856+001	1,27504186+001	-4,17242376+004	-4,22681141+004	1,26155424+003
3,53596911+001	7,18159530+005	7,22539148+005	2,52423456+003	2,49832705+001	2,68407568+001
3,14382825+003	1,04139365+002	7,24863179+002	4,74730097+000	7,73192340+000	1,39716121+001
3,06022804+002	1,35871600+001	5,15022172+001	4,28776276+001	1,59800313+000	7,34306141+000
8,61386667+000	2,08813278+003	1,74240536+002	1,32932972+001	1,46237070+002	6,60433178+002
3,00210752+001	2,42168705+001	1,46118994+001			

CLOSED SHELL F-MATRIX

-2,94807168+001	-3,919880175+001	-4,04084175+001	-1,25237666+001	-1,32048982+001	-6,09330509+000
-8,43479470+000	-9,05352866+000	-5,50165975+000	-4,63988850+000	6,36628841+003	7,49124578+003
4,11262030+003	4,39708087+003	6,44946271+000	3,78973259+003	4,33539215+003	1,01461674+002
1,42196935+002	-4,82305620+001	-1,16912569+000	1,42187036+003	1,79501111+003	1,32380774+002
2,10446217+002	-2,11424433+000	-1,64260746+000	-1,09168280+000	-3,90174705+006	6,90179954+007
2,59429580+005	-9,16098818+004	4,06446899+005	3,41230585+005	-1,46822453+002	-1,02737519+002
3,24722107+005	-8,82454159+006	-2,18912689+004	-8,64508979+004	-2,94441965+004	-3,05339931+004
-1,51165920+002	-9,38856950+001	-5,78990125+001	-6,68691382+006	3,25657109+006	3,04921738+005
-1,65686189+003	2,56749237+005	-3,86760611+005	-2,06838620+002	-3,45017716+001	-3,09239424+001
-2,07133750+001	-1,02739658+002	-1,14261478+002	-1,44293951+002	-3,06133750+002	-4,38173411+003
-1,26194476+002	-6,31088675+002	-1,48526994+000	-8,65026208+000	-4,39433733+000	-2,36183192+000
-1,97978261+001	-2,22184236+001	-2,21540054+001	-4,23644021+001	-5,35738492+002	-7,92465816+002
-1,08667712+001	-2,78900637+001	-5,42726943+001	-1,36402218+000	-1,32492048+000	-7,86368324+001
2,06272800+004	-4,03484726+005	-1,19949754+003	1,43160289+004	-1,32100128+003	-1,22175046+003
-2,87389176+003	-2,69892230+003	-2,28547105+003	-2,43295305+003	-3,10782229+003	-8,61397389+004
-1,77349935+000	-4,74244526+005	1,10528368+005	2,61219772+004	-1,51643218+003	3,06177010+004
1,94991580+004	-1,23690973+002	-1,09746669+003	-1,38598664+003	-4,64376182+003	-4,87858326+003
-2,56767012+003	-7,85780313+000	-7,49945951+000	-2,48786829+002	-2,75316597+002	-3,23913959+002
-5,79406523+002	-1,05534263+002	-2,62089230+002	-8,62276130+002	3,05624511+004	-1,81478861+003
-3,65943396+003	-2,15838564+002	-3,44253413+002	-4,47035450+000	-2,70440373+000	-1,14442354+000
-5,58249341+001	-6,22667776+001	-5,85713968+001	-3,54370365+001	-1,06433585+001	-1,47820642+001
-1,56133187+001	2,69749878+004	-1,12116773+003	-1,29368925+003	-2,39329668+002	-8,37972576+002
-3,96822647+001	-6,75019275+001	-6,28240893+001	-3,07333639+001	-3,02597022+002	-3,52053143+002
-4,74880355+002	-5,97904621+002	-2,21522992+002	-4,91497995+002	-5,89390583+002	-8,40987248+005
2,70585703+004	-6,60341796+004	-1,36895674+002	-8,90422079+002	1,73998795+003	-3,34068181+003
-3,58348022+002	-4,24030540+002	1,06763707+000	2,45469005+000	-4,77290081+001	-1,16522853+000
-2,11313170+000	-1,64314376+000	-1,09193651+000	-4,17242379+004	-4,23882406+004	1,82986412+007
-1,77412119+000	7,17884926+005	6,24327141+005	-1,43901683+003	-7,85777640+000	-7,49840339+000
-7,98612751+006	-2,02514009+003	-1,49070035+002	-2,46952434+000	-2,70263902+000	-1,12884396+000
-3,39068582+002	-4,93818294+002	-5,83805207+002	-3,96044899+001	-6,74480307+001	-6,07991646+001
-2,03290354+001	-4,79722153+003	-8,87370658+003	-4,80191000+002	1,39874638+003	-2,52202928+003
-2,46254731+002	-2,42124628+002	1,07430082+000			

TOTAL ENERGY= -6.21441505+002 HARTREES

BLOCK NO 1

VECTORS	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)
0.00000	0.9646	-0.00001	-0.00001	-0.00001	-0.00001	0.00011	0.00014	-0.00048
-0.00000	0.90706	0.00003	0.00003	0.00003	0.26463	0.00384	0.00573	-0.01427
0.00001	0.00577	-0.00044	-0.00054	-0.00054	-0.26891	-0.00891	-0.00638	0.01596
-0.00001	-0.00035	0.00068	0.00094	0.00094	-0.79897	-0.00480	-0.02773	0.08177
-0.00000	-0.80020	0.00008	0.00001	0.00001	0.00890	-0.06133	-0.00267	0.00325
0.00000	0.00009	-0.00030	-0.00007	0.00060	-0.44929	-0.02799	0.04472	
-0.00000	-0.00005	0.00038	0.00015	0.01311	-0.56472	-0.02832	0.03928	
0.85416	-0.00000	-0.23888	0.00045	-0.00011	-0.00156	0.07012	0.00608	
0.17381	-0.00000	-0.14234	0.00026	-0.00007	-0.00117	0.05220	0.00491	
0.00167	0.00001	1.08082	-0.00208	0.00057	0.00882	-0.38794	-0.03535	
-0.00019	-0.00003	0.01923	0.00074	-0.00059	-0.01711	0.81576	0.09868	
0.00007	0.00004	-0.00603	-0.00030	-0.00146	-0.00369	0.29395	-0.04570	
0.00004	-0.00001	0.00018	0.21087	0.00011	0.00072	-0.00218	0.05011	
-0.00002	0.00002	0.00140	0.81801	0.00040	0.00412	-0.01038	0.21457	
0.00000	-0.00004	0.00043	0.01640	-0.00065	-0.01082	0.02531	-0.61262	
-0.00000	0.00007	-0.00027	-0.00427	-0.00168	-0.00121	0.03607	-0.52702	
0.00000	0.00001	0.00006	0.00029	-0.00065	-0.00255	0.00812	-0.02461	
EIGENVALUES	-104.69724	-40.22669	-10.42542	-7.89250	-2.84707	-1.57087	-0.94292	-0.37003

BLOCK NO 2

VECTORS	C(1)	C(2)	C(3)
0.00006	-0.06150	-0.00052	
-0.00021	-0.24812	-0.01502	
0.00026	-0.56714	-0.00893	
0.21093	0.00012	-0.05037	
0.81808	0.00054	-0.21625	
0.01603	-0.00133	0.62141	
-0.00401	-0.00097	0.51364	
0.00023	-0.00079	0.01893	
EIGENVALUES	-7.89177	-1.56989	-0.35265

NaCl TOTAL CHARGE DENSITY

WRL 20X20 EXPOSURE

Fig. 3a. Total Charge Density of NaCl

NaCl 1S IGMV ORBITAL

WHL 20X20 EXPOSURE

Fig. 3b. 1 σ Orbital Charge Density of NaCl

NaCl 2SIGNAL ORBITAL

WHL 20X20 EXPOSURE

Fig. 3c. 2σ Orbital Charge Density of NaCl

NaCl 3SIGNAL ORBITAL

NaCl 20X20 EXPOSURE

Fig. 3d. 3 σ Orbital Charge Density of NaCl

NaCl 4s_{1/2} ORBITAL

NaCl 20020 EXPOSURE

Fig. 3e. 4s Orbital Charge Density of NaCl

NaCl 5s_{1/2} ORBITAL

WRL 20020 EXPOSURE

Fig. 3f. 5 σ Orbital Charge Density of NaCl

ACL 6SIGMA ORBITAL

WHL 20X20 EXPOSURE

Fig. 3g. 6 σ Orbital Charge Density of NaCl

NaCl 7SIGMA ORBITAL

WHL 20X20 EXPOSURE

Fig. 3h. 7 σ Orbital Charge Density of NaCl

NaCl 8 SIGMA ORBITAL

WPHL 20X20 EXPOSURE

Fig. 3i. 8 σ Orbital Charge Density of NaCl

NaCl 1 π ORBITAL

WHL 20 X 20 EXPOSURES

Fig. 3j. 1 π Orbital Charge Density of NaCl

NaCl 2 π ORBITAL

WHL 20 X 20 EXPOSURES

Fig. 3k. 2 π Orbital Charge Density of NaCl

NaCl 3 π ORBITAL

WHL 20 X 20 EXPOSURES

Fig. 31. 3 π Orbital Charge Density of NaCl

C. Input Preparation and Basis Set Choice

Much of our previous experience in building up basis sets for diatomic SCF calculations has been incorporated in an input preparation program which generates a complete input deck for BISON. This input generator is an integral part of the IBM 360/75 version of BISON and is described in Appendix E. Essentially the user is allowed to select from a table stored in the computer one of three atomic basis sets of different size for each atom of the diatomic molecule. These basis sets may, at the option of the user, be augmented with additional functions. Most of our calculations are carried out with a nominal atomic set as defined by Bagus and Gilbert with the addition and optimization of polarization functions.^{13,14} This procedure, which has been recently summarized,¹⁵ leads us to within approximately 0.001 hartree of the estimated molecular Hartree-Fock energy. Our recommendations for building up the molecular basis sets in such a manner are presented in detail in Ref. 13. The tables of the atomic functions which we customarily use are presented in Appendix F.

V. TECHNICAL INFORMATION

A. Computing Time

The time is dependent upon the basis set, the size of the grids used for the numerical integrations^{1,7} (see Sect. V-B for a discussion of the grid specifications), and to a minor extent upon the SCF iterations required for convergence. Due to input-output, and the necessity to compute tables of general coefficients and auxiliary functions, the average time per integral will decrease as the total number increases. Table 4 gives typical run times.

TABLE 4. Typical Run Times

Molecule	Number of Basis Functions	Number of Integrals		Time (min)	
		1-electron	2-electron	3600	360/75
N ₂	8	72	600	4	1.5
NaLi	26	443	20,022	90	30
NaCl	30	1056	122,256	280	88

B. Accuracy and Grid Specifications

1. The One-electron Integrals. The numerical methods¹⁰ used in the computation of the one-electron integrals results in an error of no more than 1 or 2 in the ninth significant figure, provided the suggested bias is used (NOEL). (Same grids apply to properties.)

2. The Two-center, Coulomb and Hybrid, Two-electron Integrals. The accuracy obtainable for this class of two-electron integrals depends on three factors which influence the numerical integration:^{1,7} a) the number of gaussian points used to integrate numerically over the variables ξ and η ; b) the magnitude of the orbital exponents involved in the integral; c) the internuclear and the truncation distances. The integral accuracy is not significantly dependent upon the quantum numbers of the basis functions. Table 5 indicates the grid necessary to achieve an absolute accuracy of $10^{-5} e^2/\text{Bohr}$. (Accuracy to 9 significant figures can be obtained by increasing grids if desired.)

3. The exchange integrals have a fixed accuracy of better than $10^{-6} e^2/\text{Bohr}$. This accuracy is assured for all types of exchange integrals by the use of a 50-point Simpson integration and 10 Neumann iterations.

The choice of RMAX is given in the input specifications. The above specifications are intended as a reasonable guide. If the user intends to use this program for an extensive series of integral calculations, we

suggest that he first investigate the convergence characteristics of the total energy over his own particular basis set in order to arrive at the most economical but sufficient grid parameters. The time per integral is roughly proportional to the total number of integration points used.

TABLE 5. Numerical Grids for Integral Evaluation

Maximum Orbital Exponent in Basis Set	Grid Necessary ^a			
	R	Points on ξ	Points on η	R _{Max}
3.0	2.0	12	12	16
3.0	12.0	12	20	20
9.0	3.6	24	20	20
15.0	3.6	24	24	20
15.0	12.0	30	30	20

^aLarger grids can be used for greater accuracy.

4. The One-center Two-electron Integrals are computed analytically and are accurate to 9-10 significant figures.

VI. PROGRAM STRUCTURE

A. Language

The program is entirely coded in FORTRAN, for a CDC-3600 multichannel disk-tape or all-tape machines with 64k core and an IBM-360/75 with disks and 10^6 bytes of fast memory. The CDC-3600 program was compiled and constructed using the ANL scope but can be compiled with any minimal scope, i.e., 6.1. The IBM-360/75 version was compiled in FORTRAN H optimization level 2. The program also has been adapted to CDC-3600 with 32k core.

B. Overlay Design

The program currently consists of 10 separate overlays (see Fig. 4).

The executor is the overseer and driver for all computations.

Fig. 4. Overlay Tape Structure

Once loaded, the executor remains in the core throughout all the computations. The input is read, screened, and loaded into the data blocks. The executor then calls the appropriate overlays sequentially into core. Upon completion of a "run," the executor calls into core the input driver, which looks for a new set of input, which if present, is read in. The cycle is then repeated until all the input data are exhausted, and at that point the job is terminated.

Once the executor has been loaded, the program is completely automatic and self-diagnostic. It has been designed in this fashion to minimize the possibility of costly time-consuming errors and to fit into a normal schedule requiring no special operator activity.

C. Limitations

The program has several inherent limitations, some of which may be relaxed. These limitations are:

1. The program is operative on a CDC-3600 multichannel, disk-tape or all-tape machine with 64k memory or on an IBM-360/75 with 1 megabyte core.
2. The program uses a total of 10 tapes (CDC-3600) or data sets (IBM-360/75).
3. The maximum number of supermatrix elements permitted is 1,500,000. This can be expanded but most "feasible" diatomics of interest fall well within this limitation.
4. The maximum size of the basis set is limited by the supermatrix size. The number of basis functions permitted, however, varies depending upon their distribution among various symmetrics.

The following relationships define the total number of one- and two-electron integrals and supermatrix elements arising over a given number of basis functions.

One-electron Integrals (per operator) N_0

$$N_0 = \sum_{\lambda} \frac{n_{\lambda}(n_{\lambda} + 1)}{2}$$

where

N_0 = total number of integrals;

n_{λ} = number of basis functions in symmetry λ .

Supermatrix Elements (J , K^+ or K^-)

$$N_s = N_0(N_0 + 1)/2.$$

5. The quantum numbers must always be integers and fall within the following ranges:

$$1 < n \leq 8; \quad \ell \leq n - 1; \quad |m| \leq \ell.$$

Zeta can be any decimal number in the range $0.01 < \zeta < 100$.

6. The program can be used only as a self-contained independent program. No provision has been made for its use as a closed subroutine.

D. Core-space Allocations, Tape, and Disk Commitments

The following are the current storage commitments of the program.

1. Core Allocations:

(CDC-3600) SCOPE System--14,000 words; programs and working space, 50,000 words.

(IBM-360/75) System--200,000 bytes; program and working space, 800,000 bytes.

2. Tape Assignments

a) Two-channel CDC-3600:

Tape 21	Overlay tape containing program
Tape 60	Output tape
Tape 40 J	Supermatrix
Tape 41 K ⁺	Supermatrix
Tape 42 K ⁻	Supermatrix
Tape 49 S, U, and T matrices	

52

53

SCRATCH TAPES

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55

b) IBM-360/75 version uses only one tape when saving of integrals is requested. Entire program is stored on disks, and disks are heavily used during integral generation.

E. Flow Charts of Program

FLOW CHART OF EXECUTOR

FLOW CHART FOR JEX

FLOW CHART FOR JCH

FLOW CHART FOR KEX

FLOW CHART FOR KCH

FLOW CHART FOR P2

FLOW CHART OF SCF

FLOW CHART OF MOLECULAR PROPERTIES

FLOW CHART OF CONTOUR PLOTTING

VII. APPENDICES

A. Construction of the Program Tape or Disk File

The CDC-3600 overlay tape is constructed through the normal overlay feature of SCOPE (see SCOPE Reference Manual). The IBM-360/75 program is constructed using the overlay feature and placed as a partitioned data set on disk.

B. Summary

Name:	BISON
Purpose:	To compute self-consistent-field wavefunctions, properties, and charge densities for diatomic molecules.
Language:	FORTTRAN: CDC FORTRAN; IBM FORTRAN IV
Source Deck:	6000 FORTRAN statements
Hardware:	CDC-3600: 64k, 16 tapes; IBM-360/75: 10 ⁶ bytes, sixteen 2314 disks, four 9-track tapes.
Library Routines Referred to:	Standard FORTRAN
Number of Words Used:	CDC-3600: 64k, 10 overlays; IBM-360/75: 128k (8 byte words, 10 overlays).
Program Stops:	None except error stops.
Running Time:	IBM-360/75: 1½ min for the calculation of SCF function for minimum basis set (8 basis functions) for N ₂ . NaCl: 1½ hr (30 basis functions).
Special Features:	<ol style="list-style-type: none"> 1. Program entirely on tape or disk (IBM) 2. Loaded using Loadmain (CDC); EXEC PGM = Driver (IBM) 3. Overlaid 4. Automatic and self-diagnostic 5. Output may be printed, punched, or written on magnetic tape. 6. Writeup available 7. Double Precision on IBM-360/75 version
Job Termination:	<ol style="list-style-type: none"> 1. Normal; by signifying end of data with end-of-run card, terminates if unrecoverable input-output errors occur.
Restrictions:	<ol style="list-style-type: none"> 1. STO Basis 2. Matrix Elements: 1000 3. 1,500,000 Supermatrix Elements 4. $n \leq 8$; $\ell \geq n - 1$; $m < \ell$

- Accuracy:** All results may be obtained accurate to nine significant figures.
- Abstract:** Techniques and a new computer program developed by the authors for obtaining self-consistent-field (SCF) wavefunctions and properties [very close to the Hartree-Fock (HF) limit] via the Roothaan Expansion Method for heteropolar or homopolar diatomic molecules containing atoms from rows 1 through 5 of the periodic table are discussed.
- The computer program, which is written entirely in FORTRAN, evaluates all necessary integrals, performs the SCF procedure and then computes charge-density contours and a variety of molecular properties from the resulting SCF wavefunction. The limitations on the quantum numbers of the Slater-type orbital (STO) basis are $1 \leq n \leq 8$; $0 \leq \ell \leq n - 1$; $-\ell \leq m \leq \ell$; a maximum of $1\frac{1}{2}$ million supermatrix elements are permitted which allows accurate SCF calculations on very large diatomic systems. Typical results of recent extended basis-set calculations for the alkali halide NaCl, which illustrate program usage, are presented.
- References:** Wahl, A. C., J. Chem. Phys. 41, 2600 (1964);
Wahl, A. C., Cade, P. E., and Roothaan, C. C. J., J. Chem. Phys. 41, 2578 (1964);
Wahl, A. C., Bertoncini, P. J., Das, G., and Gilbert, T. L., Int. J. of Quantum Chem. 1S, 123 (1967)
- Authors:** A. C. Wahl, P. J. Bertoncini, and K. Kaiser, Chemistry Division; and Robert H. Land, Solid State Science Division, Argonne National Laboratory.

C. Supplement for 8-tape, 64k CDC-3600

1. Input and output are as previously described.
2. Tape commitments are as follows:
 - a) Scope on standard unit.
 - b) Input on standard unit.
 - c) Output on on-line printer (or output tape if input from card reader).
 - d) BISON unit 21.
 - e) J produced on unit 40 and saved until P and Q constructed. Then S , U , and T are placed and saved on unit 40. Tape 40 should be saved.
 - f) Units 41-44 used in construction of K^+ , K^- , P , and Q supermatrices.
 - K^+ will be on either unit 43 or 44
 - K^- will be on either unit 41 or 42

P will be on either unit 41 or 42
 Q will be on either unit 43 or 44

The output will state which supermatrix is on which tape.
 These four tapes, 41-44, should be saved and then the two
 unwanted tapes released after the run.

- g) In order to utilize the scope scratch tape the statement
 7 Equip, 40 = 50 should precede Loadmain card.

3. Control cards for CDC at Centre de Mechanique Ondulatoire
 Applique, 27 rue du Maroc, Paris:

7 Job, MOA 167, Name, Time

7 Equip, 21 = (BISON ... 999), SV, RO

7 Equip, 40 = 50

Proper Equip statements
 as described in 4.

7 Loadmain, 21

4. If run is made from previously computed integral tapes, then
 the following assignments must be made depending upon where the calcu-
 lational sequence begins.

- a) Starting with SCF process
 P on unit 42
 Q on unit 44
 S.U.T. on unit 40 (this was SCOPESCRATCH tape)
- b) Starting with construction of P and Q from previously
 produced J, K^+ , and K^- :
 J on unit 40
 K^+ on unit 43
 K^- on unit 41
- c) Starting with construction of K^+ and K^- :
 J on unit 40.

Since, in general, the supermatrices P, Q, K^+ and K^- will
 not be produced on above unit, they must be equipped to be
 on these units at the beginning of the run.

D. Supplement Describing Operation of Program on a 32k CDC-3600

Input is the same as standard version.

Output is the same as standard version.

Two additional tape units are required for the handling of electro-
 static coulomb and exchange potentials.

E. Supplement Describing Operation of Program on an IBM-360/75

1. Format of the Data Module for the IBM-360/75 Version of BISON

The general structure of the BISON data module is as follows:

Section (A). Four cards which enter the title, molecular constants, grid sizes for the numerical integrations, and control flags for the program.

Section (B1) or Section (B2). A set of cards for each symmetry block which enter the orbitals, the quantum numbers and orbital exponents, and the vector components for each occupied orbital. Two different methods are provided for entering the data for the symmetry blocks. The data may be entered explicitly using the format for section (B1) of the data module or the data may be taken from a disk file in which are stored basis sets for atoms with atomic number ≤ 36 . In this latter case, the format for section (B2) of the data module is used. A catalog of this disk file is provided in Appendix F for use in preparing section (B2) of the data module.

Section (C). The cards in section (C) enter the vector coupling coefficients. These coefficients are needed only if open shells are present. This section is followed by an end of run card.

All numbers used in this data module are punched using a generalized format, i.e., they may be in the I, F, E, or D format. These constants are to be entered on the appropriate cards in the order specified and separated by any number of blank card columns. The blank card columns thus act as delimiters for the various constants punched on the cards. Note that since blanks are used as delimiters, constants which have the value zero must be entered as zero and not left blank.

The data module is thoroughly screened by the program to prevent costly erroneous calculations. A detailed description of each section of the data module follows.

Section (A)

	FORTTRAN Symbol	Description
Card 1	Title	Entire card may be used for a title (Format = 10A8), e.g., CA ϕ NOMINAL BASIS SET.
Card 2	RR RMAX	Internuclear distance in Bohrs. This truncates the upper limit in the numerical integrations. RMAX may be computed by the following equation: $RMAX \approx 60.0/2 \zeta_{MIN}$ where ζ_{MIN} is the smallest orbital exponent in the basis set.

	FORTTRAN Symbol	Description
Card 2 (Contd.)	NXI	The number of Gauss points on Xi and Eta respectively, used in the Gaussian numerical integration section of the coulomb-hybrid programs. Suggested values are 30. The allowed grid sizes are 12, 16, 20, 24, 30, 36, 40, 50, 60, 70, 80, 90, and 100. If the requested grid is different than those in stock, the program will substitute the grid size nearest to the requested size. See Sect. V-B for grid specifications.
	NETA	
	NDUM	
	MDUMF	
	ZA	
	ZB	Nuclear charge on center B.
Card 3	NNEU	Number of Neumann iterations employed. Suggested value 10. Maximum permitted 40.
	NSIMP	Specifies the number of Simpson rule points used in the numerical integration section of the exchange programs. Suggested value 50. NSIMP is restricted to the range $0 \leq \text{NSIMP} \leq 95$. See Sect. V-B for grid specifications.
	NBIAS	Bias for one electron matrix integration, suggested value 20.
Card 4	IOPEN	Open shell flag 1 for open shell calculations 0 closed shells only
	IVECT	SCF printing flag 0 suppresses all print but for final iterations 1 prints all iterations and extrapolations
	IPRINT	Integrals print flag 1 S, U, T, H, F and supermatrices will be printed 0 only S, H, and F are printed
	KFLG	Calculation option flag--specifies at what stage the diatomic calculation is to be started (KFLG) ended (JFLG)
	JFLG	
		0 do entire calculation
		1 { start with input loading and screening end,
		2 { start with J exchange integrals end, put J_{ex} on tape if ISAVE = 1

	FORTTRAN Symbol	Description
Card 4 (Contd.)	KFLG JFLG (Contd.)	<p>3 { start with J coulomb-hybrid integrals end, put J on tape if ISAVE = 1</p> <p>4 { start with K exchange integrals end, put K_{ex}^+, K_{ex}^- on tape if ISAVE = 1</p> <p>5 { start with K coulomb-hybrid integrals end, put K^+, K^- on tape if ISAVE = 1</p> <p>6 { start with S, U, and T end, put S, U, T on tape if ISAVE = 1</p> <p>7 { start with construction of P and Q and do SCF procedure. Read in J, K^+, K^-, S, U and T from tape. end save J, K^+, K^-, S, U, T on tape if ISAVE = 1.</p> <p>8 { same as 7 except J, K^+, K^-, S, U, and T must already be on disk.</p> <p>9 { start with calculation of molecular properties end</p> <p>10 { start with plotting of orbital and total charge density contours end</p>
	IPRCT	Prior SCF iterations before extrapolations are begun. Suggested value 5.
	ISCF	Negative power of 10 for the SCF threshold. The SCF process is terminated when the differences between all vector components from two successive iterations is less than this power of 10. Suggested values ISCF = 3, i.e., 0.001 (very loose) ISCF = 7, i.e., 0.0000001 (tight) usually ISCF = 5, i.e., 0.00001 yields the desired accuracy in the vectors.
	ICH	Negative power of 10 for the convergence threshold for calculation of electrostatic potentials in integrals com- putation. A value of ICH = 7, i.e., 0.0000001 is suggested.
	IPUNCH	0 no punched output 1 input deck in (B1) form is punched along with the final vectors
	IDEBUG	1 prints out intermediate data for "debugging" 0 no intermediate data printed
	INFLG	0 section (B) of data module is in (B1) format 1 section (B) of data module is in (B2) format
	ISAVE	0 no integrals put on tape 1 save integrals on tape

END OF SECTION (A)

Section (B) use either (B1) or (B2) but not both

Section (B1)

	FORTTRAN Symbol	Description
Card 1	NLAMDA	The number of basis functions in the current symmetry block.
	NORBS	The number of occupied orbitals in the current symmetry block.
	NC	The number of closed shell orbitals in the current symmetry block.
	NØ	The number of open shell orbitals in the current symmetry block.
Card 2	CM	The closed shell occupation numbers, NLAMDA of these are stored by the program. Nonzero value of n^{th} CM indicates n^{th} orbital occupation in the current symmetry. The CM's need to be punched until all occupied orbitals are entered, then the program will fill the rest of the CM's with zeros. More than one card may be used if desired.
Card 3	CM	Open shell occupation numbers, not necessary if closed shell case (IOPEN = 0). Format as in Card 2. This card must be present if IOPEN = 1.
Card 4.1 to Card 4.NLAMDA	N L M ZETA	The quantum numbers n, l, m of the basis function and the orbital exponent ζ . ζ is + if on center A, ζ is - if on center B. There is one card for each basis function.

	FORTTRAN Symbol	Description
Vector Component ₁ { Card 5.1.1 to 5.1.NLAMDA	CIP	Vector Components. NLAMDA cards are given for each occupied orbital. First for the closed shells and then for the open. If a CIP is zero a blank card may be entered.
Vector Component ₂ { Card 5.2.1 to 5.2.NLAMDA		
Vector Component NORBS { Card 5.NORBS.1 to Card 5.NORBS.NLAMDA		
Card 6 (For last symmetry block only)		This card is blank if the current symmetry block is the last one. If not, a new block is entered starting with Card 1 of this section.

END SECTION (B1)

Section (B2)*

*Note--Alphameric data fields used in this section must be delimited by blanks.

	FORTTRAN Symbol	Description
Card 1.	ATMTAG(1) ATMTAG(2)	The label of the atomic basis set taken from the disk file catalog, first for center A then for center B. E.g., LI+(1S)N and F-(1S)N.

	FORTTRAN Symbol	Description
Card 2	LET(1) NLAMDA NORBS NC NØ	Symmetry, i.e., the word SIGMA, PI, or DELTA. The description for these four variables is the same as that given in section (B1) for Card 1. Note that NLAMDA should include any augment functions specified on Cards 3 and 4. Also NORBS should include any EXTERN'S specified on Card 5.
Card 3 (optional)	LET(1) AUGTAG NAUG	If you wish to augment the disk basis set for an atom, enter a card with AUGMENT in card columns 1 to 7. The atom whose basis set is to be augmented. Enter all of alphameric characters before the first parenthesis in the atom label. E.g., for LI+(1S)N enter LI+. The number of basis functions to be added to the original set on the disk.
Card 4 (optional)	LET(1) AUGTAG NAUG	If you wish to augment both atomic basis sets enter this card for the second atom. The format is the same as Card 3.
Card 5	ORBTAG	Enter the labels for the orbitals in the order desired. More than one card may be used if necessary. The orbital labels should be taken from the disk file catalog, mentioned above. If it is desired to enter vector components for an orbital which is not on the disk, enter the label EXTERN in the appropriate place on this card.

	FORTTRAN Symbol	Description
Card 6	CM	The closed shell occupation numbers. The format is the same as Card 2, section (B1).
Card 7	CM	Open shell occupation numbers, not necessary if closed shell case (IOPEN = 0). The format is the same as Card 3, section (B1). This card must be present if IOPEN = 1.
Card 8.1 to Card 8.NAUG (optional)	N L M ZETA	The NAUG basis functions referred to in Card 3. The format is given under Card 4, section (B1). Punch one (N, L, M, ZETA) set per card.
Card 9.1 to Card 9.NAUG (optional)	N L M ZETA	The NAUG basis functions referred to in Card 4. The format is given under Card 4, section (B1).
First EXTERN {	Card 10.1.1 to Card 10.1.NLAMDA	CIP
Last EXTERN {	Card 10. η .1 to Card 10. η .NLAMDA	Vector component for each EXTERN listed on Card 5. C.f. Card 5, section (B1). If a CIP is zero a blank card may be entered. η = number of EXTERN's on Card 5.
	Card 11 (For last symmetry block only)	This blank card is entered if the current symmetry block is the last one. If not, a new block is entered starting with Card 2 of this section.

END SECTION (B2)

Section (C)

	FORTTRAN Symbol	Description
Card 1.1 to Card 1.NCDS	ALPHA BETAP BETAM	The $A_{\lambda\mu}$, $B_{\lambda\mu}$, $C_{\lambda\mu}$ vector coupling coefficients for the open shell cases. Needed only if open shells are present. Each card contains three coefficients--A, B, and C. See Table 3a for values. If NSYM equal the number of symmetry blocks entered in section (B1) or (B2), then $3(NSYM)(NSYM+1)/2$ vector coupling coefficients or $(NSYM)(NSYM+1)/2 = NCDS$ cards must be entered. The order of the cards is: A_{11}, B_{11}, C_{11} A_{12}, B_{12}, C_{12} A_{22}, B_{22}, C_{22} A_{13}, B_{13}, C_{13} A_{23}, B_{23}, C_{23} A_{33}, B_{33}, C_{33} . . .
Card 2 (only if last data module)		Enter a new data module or if last data module enter this card with END OF RUN in card columns 1-10.

END SECTION (C)

2. Job Control Language Information for IBM-360/75 as Used by the BISON SystemI. Introduction to JCL[†]A. Rules for Coding JCL Statements

1. Job control statements are identified by the characters // or /* in card columns 1 and 2 and may contain three fields: a name, operation and operand field. One or more blanks are used to separate the fields. The blanks are delimiters on JCL cards. Thus the occurrence of a blank in a field causes the system to scan for the next field. Unnecessary blanks can thus cause JCL errors to prevent successful running of a job.

[†]For more complete description of Job Control Language see IBM System/360 Operating System: Job Control Language C28-6539; IBM System/360 Operating System: FORTRAN (H) Programmer's Guide.

a. Name Field

i. This field is optional. Its absence must be indicated by at least one blank. The name can contain up to eight alphameric characters, the first of which must be alphabetic. The name field begins in column 3 and is followed by one or more blanks.

b. Operation Field

i. The operation field contains one of the following operation codes:

JOB
EXEC
DD

ii. The operation field is ended by a blank.

c. Operand Field

i. The operand field contains the parameters that provide required and optional information to the operating system. Parameters are separated by commas and the operand field is ended by blanks after the last parameter.

2. A control statement may occupy card columns 1 through 71. If a control statement exceeds 71 columns, it may be continued into the next card. If a control statement is continued, it must be interrupted after the comma that follows the last parameter on the card and a nonblank character placed in column 72. The continuation card must contain // in columns 1 and 2, columns 3 through 15 must be blank, and the continued portion of the statement must begin in column 16. There is no limit to the number of continuation cards used for a single control statement.

3. Examples

a. //Name Operation Operand

b. //Molecule JOB (accounting information), Programmer's Name

c. //Go EXEC PGM=BISØN

d. //FT07FOO1 DD UNIT=(SYSCP,,DEFER)

e. /*Setup DDNAME=JOBLIB,DEVICE=2314,ID=DISK12.

B. Sample JCL Statements for BISON Jobs

1. Basic JCL Deck

a. Sample of JCL deck structure for complete integrals and SCF run, integrals not saved.

```

EXAMPLE 1a
//MOLECULE JOB (badge#,linelimit,card limit,time limit),programmer'sname,X
//          MSGLEVEL=1
ACCOUNTING CARD
/*SETUP DDNAME=JOBLIB,DEVICE=2314,ID=DISK12
//JOBLIB DD DSN=JOBLIB,LOADMOD=SER=DISK12,
//          DISP=(OLD,PASS)
          (The following cards scratch disks SCRONE and SCRTWO)

//ERASE EXEC PGM=IEHPRGM
//SYSPRINT DD SYSOUT=A
//DD1 DD UNIT=DISK,VOLUME=SER=SCRONE,DISP=OLD
//DD2 DD UNIT=DISK,VOLUME=SER=SCRTWO,DISP=OLD
//SYSIN DD *
          SCRATCH VTOC,VOL=2314=SCRONE,PURGE } THESE CARDS ARE
          SCRATCH VTOC,VOL=2314=SCRTWO,PURGE } IEHPRGM INPUT CARDS
/*

          (The following cards are control cards for the execution of BISON)

//GO EXEC PGM=BISON
//FT05F001 DD DDNAME=SYSIN
//FT06F001 DD SYSOUT=A,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=798)
//FT07F001 DD UNIT=(SYSCP,,DEFER)
//FT56F001 DD UNIT=DISK,VOLUME=SER=DISK12,DISP=OLD,DSNAME=BISON.INPUT
//FT40F001 DD DSN=JOBLIB.MOLECULE,UNIT=DISK,VOLUME=SER=DISK12,
//          DISP=OLD
//FT41F001 DD DSN=JOBLIB.KPSUP.MOLECULE,UNIT=DISK,VOLUME=SER=DISK12,
//          DISP=OLD
//FT42F001 DD DSN=JOBLIB.KMSUP.MOLECULE,UNIT=DISK,VOLUME=SER=DISK12,
//          DISP=OLD
//FT49F001 DD DSN=JOBLIB.SUT.MOLECULE,UNIT=DISK,VOLUME=SER=DISK12,
//          DISP=OLD
//FT51F001 DD UNIT=DISK,VOLUME=SER=SCRONE,DISP=(NEW,DELETE),
//          SPACE=(CYL,(30,2)),DCB=(RECFM=VB,LRECL=918,BLKSIZE=2758)
//FT52F001 DD UNIT=DISK,VOLUME=SER=SCRTWO,DISP=(NEW,DELETE),
//          SPACE=(CYL,(30,2)),DCB=(RECFM=VB,LRECL=918,BLKSIZE=2758)
//FT53F001 DD UNIT=DISK,VOLUME=SER=SCRTWO,DISP=(NEW,DELETE),
//          SPACE=(CYL,(30,2)),DCB=(RECFM=VB,LRECL=918,BLKSIZE=2758)
//FT54F001 DD UNIT=DISK,VOLUME=SER=SCRONE,DISP=(NEW,DELETE),
//          SPACE=(CYL,(30,2)),DCB=(RECFM=VB,LRECL=918,BLKSIZE=2758)
//FT77F001 DD UNIT=DISK,VOLUME=SER=DISK12,DISP=OLD
//          DSN=JOBLIB.ATOMIC.SCF.INPUT
//SYSIN DD *
          Input decks for BISON
/*

```

b. If space has not been assigned on DISK12 for FOTRAN data sets FT40, FT41, FT42, and FT49, space must be requested by use of the DD card SPACE and DCB parameters similar in format to those used in the FT51 etc. DD cards. Care should be taken not to request more space than necessary since DISK12 will then become cluttered up with data sets which fill only a fraction of the space allotted. A cylinder on the 2314 disk will contain roughly 18,000 double precision words. The DISP parameter on the DD card must specify (NEW,KEEP) in order to create and keep the data sets. For example, for FT40

EXAMPLE 1b

```
//FT40F001 DD DSN=JSUP.MOLECULE,UNIT=DISK,VOLUME=SER=DISK12,      X
//          SPACE=(CYL,(7,2)),DCB=(RECFM=VB,LRECL=918,BLKSIZE=2758), X
//          DISP=(NEW,KEEP)
```

2. Save integrals on tape for three sets of input.

a. Add cards below to standard deck setup from Example 1.

EXAMPLE 2a

```
/*SETUP DDNAME=FT43F001,DEVICE=2400-9,ID=(,RING,SAVE,SL)
      (add after /*SETUP DDNAME=JOBLIB,... )
.
.
.
//FT43F001 DD UNIT=TAPE,DSNAME=datasetname1,LABEL=(1,SL),DISP=(,KEEP)
//FT43F002 DD UNIT=TAPE,DSNAME=datasetname2,LABEL=(2,SL),DISP=(,KEEP),  X
//          VOLUME=REF=*.FT43F001
//FT43F003 DD UNIT=TAPE,DSNAME=datasetname3,LABEL=(3,SL),DISP=(,KEEP),  X
//          VOLUME=REF=*.FT43F001
      (add the above cards before FT40F001 DD card)
.
.
.
//SYSIN DD *
      3 sets of input data corresponding to files 1, 2, and 3
      of tape.
/*
```

b. When submitting job with setup card /*SETUP as shown, submit a tape save request. If a particular library tape is to be used, submit a deck with the following setup card.

EXAMPLE 2b

```
/*SETUP DDNAME=FT43F001,DEVICE=2400-9,ID=(XXXXXX,RING,SAVE,SL)
```

i. Where in ID=(XXXXXX,RING,SAVE,SL),XXXXXX is the five digit library number on the tape save request. This five digit number is preceded by a zero to give the six digit ID number.

3. Read integrals from tape from the third file of the tape to do SCF calculation.

a. Use standard deck structure and add the following cards similar to those of Examples 2a and 2b.

EXAMPLE 3

```
/*SETUP DDNAME=FT43F001,DEVICE=2400-9,ID=(XXXXXX,RING,SAVE,SL)
```

```
      . (STANDARD JCL DECK SEE EXAMPLE 1)
```

```
//FT43F001 DD UNIT=TAPE,DSNAME=datasetname3,LABEL=(3,SL),DISP=(,KEEP)
```

```
      . (STANDARD JCL DECK SEE EXAMPLE 1)
```

```
//FT05F001 DD *
```

```
      . Input data corresponding to data set name 3 of file 3 of tape XXXXXX
/*
```

b. It should be understood that in writing the tapes file 1 should be written before file 2, etc., i.e., the FORTRAN sequence # F001 should be the same as the data set sequence # in LABEL=(N,SL). In reading the tape, the files can be read in any order. The FORTRAN sequence # F001 is used for the first read and may correspond to reading file 3 by LABEL=(3,SL). The second read uses F002 and can read any file, file 1 for example, by the use of LABEL=(1,SL).

4. It will become obvious to the user as he becomes more proficient in JOB CONTROL LANGUAGE, that many options and possibilities are open to him in the assigning of units, saving of data sets, use of nonstandard input and output devices, and concatenation of data sets which are only hinted at here.

a. A few cautious notes ought to be sounded at this time.

i. At present, data sets FT40, FT41, and FT42 must be located on a disk or drum.

ii. The allocation of space for these data sets on the disk should not be too generous if space is not to be wasted on the disk, since space once allocated cannot be used if unfilled except by scratching the data sets or by use of the RLSE subparameter in the SPACE parameter.

2	1	1	10.23200	
2	1	1	6.71500	
3	1	1	3.52700	
3	1	1	2.20300	
3	2	1	2.69460	
3	2	1	0.69740	
2	1	1	-4.61800	
2	1	1	-2.25400	
2	1	1	-0.99400	
3	2	1	-2.49000	
3	2	1	-1.09000	
0.02750				
0.29673				
0.70286				
0.00870				
-0.00175				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
-0.00898				
-0.08393				
-0.26706				
0.61542				
0.49520				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.0				
0.13091				
0.56376				
0.44284				
0.0				
0.0				
1.00000000	-0.25000000	-0.25000000		
0.0	0.08333333	0.08333333		
0.11111111	-0.02777778	-0.02777778		

END OF RUN

SAMPLE DATA MODULE FOR BISON--OPTION (B2)

CAO- NOMINAL BASIS SET 3-PI
 3.52 30 30 30 0 0 20 8
 10 50 20
 1 1 0 1 1 5 5 7 1 0 1 0
 CA(1S)N 0-(1S)N
 SIGMA 24 9 8 1
 AUGMENT CA 2
 AUGMENT O- 2
 1SCA 1SO- EXTERN 2PCA 3SCA 3PCA 2SO- 2PO- 4SCA
 2 2 2 2 2 2 2 2
 0 0 0 0 0 0 0 1
 3 2 0 2.6946
 3 2 0 .6974
 3 2 0 2.49
 3 2 0 1.09
 0.26108
 0.14103
 -0.06108
 -1.03766
 -0.01636
 0.00543
 -0.00103
 0.00036
 -0.00008
 -0.00017
 -0.00079
 0.00013
 0.00016
 0.00003
 -0.00002
 0.00000
 -0.00000
 0.00005
 -0.00003
 0.00002
 -0.00003
 -0.00008
 -0.00002
 -0.00011
 PI 12 3 2 1
 AUGMENT CA 2
 AUGMENT O- 2
 2PCA 3PCA 2PO-
 4 4
 0 0 3
 3 2 1 2.6946
 3 2 1 .6974
 3 2 1 2.49
 3 2 1 1.09
 1. -.25 -.25
 0 .08333333 .08333333
 .11111111 -.02777778 -.02777778
 END OF RUN

BISON
Computing System for the Calculations of Wavefunctions and
Properties of Diatomic Molecules
by A. C. Wahl, P. J. Bertoncini, and K. Kaiser, Chemistry Division,
and R. H. Land, Solid State Science Division,
Argonne National Laboratory
June 18, 1968

CAC NOMINAL BASIS SET I 3-PI

ZA = 20.000 ZB = 8.000

INTERNUCLEAR DISTANCE = 3.5200 BOHRS

NUMBER OF GAUSS POINTS ON XI = 30

INTEGRATION TRUNCATED AT 30.0000 BOHRS

NUMBER OF GAUSS POINTS ON ETA = 30

NUMBER OF NEUMANN ITERATIONS = 10

NUMBER OF SIMPSONS POINTS = 50

BIAS FOR ONE ELECTRON GRID = 20

VECTOR COEFFICIENT DIAGONALIZATION THRESHOLD = 1.0000-05

PRICR ITERATIONS = 5

CCOLGME-HYBRID CONVERGENCE THRESHOLD = 1.0000-07

CENTER A = C(15)N CENTER B = C-(15)N

BASIS SET BLOCK I

CENTER

ORBITAL COEFFICIENTS

N	L	M	ZETA		1SCA C(11)	1SO- C(12)	EXTERN C(13)	2PCA C(14)	3SCA C(15)	3PCA C(16)	2SO- C(17)	2PO- C(18)	4SCA C(19)
1	0	0	21.12500	A	0.89911	0.0	0.26108	0.0	0.08990	0.0	0.0	0.0	-0.02146
2	0	0	18.25300	A	0.12409	0.0	0.14103	0.0	0.06960	0.0	0.0	0.0	-0.01756
3	0	0	12.86700	A	-0.00688	0.0	-0.06108	0.0	0.04659	0.0	0.0	0.0	-0.01472
2	0	0	7.33200	A	0.00559	0.0	-1.03766	0.0	-0.55278	0.0	0.0	0.0	0.14093
3	0	0	3.67400	A	-0.00177	0.0	-0.01636	0.0	0.72517	0.0	0.0	0.0	-0.21081
3	0	0	2.94500	A	0.00118	0.0	0.00543	0.0	0.41276	0.0	0.0	0.0	-0.09695
4	0	0	1.45500	A	-0.00034	0.0	-0.00103	0.0	-0.00238	0.0	0.0	0.0	0.50157
4	0	0	0.87500	A	0.00014	0.0	0.00036	0.0	0.00081	0.0	0.0	0.0	0.60261
2	1	0	17.00000	A	0.0	0.0	-0.00008	0.02750	0.0	-0.00898	0.0	0.0	0.0
2	1	0	10.23200	A	0.0	0.0	-0.00017	0.29673	0.0	-0.08393	0.0	0.0	0.0
2	1	0	6.71500	A	0.0	0.0	-0.00079	0.70286	0.0	-0.26706	0.0	0.0	0.0
3	1	0	3.52700	A	0.0	0.0	0.00013	0.00870	0.0	0.61542	0.0	0.0	0.0
3	1	0	2.20300	A	0.0	0.0	0.00016	-0.00175	0.0	0.49520	0.0	0.0	0.0
3	2	0	2.69460	A	0.0	0.0	0.00003	0.0	0.0	0.0	0.0	0.0	0.0
3	2	0	0.69740	A	0.0	0.0	-0.00002	0.0	0.0	0.0	0.0	0.0	0.0
1	0	0	11.99600	B	0.0	0.07660	0.0	0.0	0.0	0.0	-0.00841	0.0	0.0
1	0	0	7.32600	B	0.0	0.92790	0.0	0.0	0.0	0.0	-0.22281	0.0	0.0
3	0	0	4.32400	B	0.0	0.00557	0.00005	0.0	0.0	0.0	0.34067	0.0	0.0
2	0	0	1.82400	B	0.0	-0.00038	-0.00003	0.0	0.0	0.0	0.72898	0.0	0.0
2	1	0	4.61800	B	0.0	0.0	0.00002	0.0	0.0	0.0	0.0	0.13091	0.0
2	1	0	2.26400	B	0.0	0.0	-0.00003	0.0	0.0	0.0	0.0	0.56376	0.0
2	1	0	0.59400	B	0.0	0.0	-0.00008	0.0	0.0	0.0	0.0	0.44284	0.0
3	2	0	2.49000	B	0.0	0.0	-0.00002	0.0	0.0	0.0	0.0	0.0	0.0
3	2	0	1.09000	B	0.0	0.0	-0.00011	0.0	0.0	0.0	0.0	0.0	0.0

NUMBER OF ELECTRONS OCCUPYING
CLOSED SHELL ORBITALS = 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 0.0

NUMBER OF ELECTRONS OCCUPYING
OPEN SHELL ORBITALS = 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0

BASIS SET BLOCK II

CENTER

ORBITAL COEFFICIENTS

N	L	M	ZETA		2PCA C(11)	3PCA C(12)	2PO- C(13)
2	1	1	17.00000	A	0.02750	-0.00898	0.0
2	1	1	10.23200	A	0.29673	-0.08393	0.0
2	1	1	6.71500	A	0.70286	-0.26706	0.0
3	1	1	3.52700	A	0.00870	0.61542	0.0
3	1	1	2.20300	A	-0.00175	0.49520	0.0
3	2	1	2.69460	A	0.0	0.0	0.0
3	2	1	0.69740	A	0.0	0.0	0.0
2	1	1	4.61800	B	0.0	0.0	0.13091
2	1	1	2.26400	B	0.0	0.0	0.56376
2	1	1	0.59400	B	0.0	0.0	0.44284
3	2	1	2.49000	B	0.0	0.0	0.0
3	2	1	1.09000	B	0.0	0.0	0.0

NUMBER OF ELECTRONS OCCUPYING
CLOSED SHELL ORBITALS = 4.0 4.0 0.0

NUMBER OF ELECTRONS OCCUPYING
OPEN SHELL ORBITALS = 0.0 0.0 3.0

VECTOR COUPLING COEFFICIENTS

A(1,1)= 1.0000000	B(1,1)= -0.25000000	C(1,1)= -0.25000000
A(2,1)= 0.0	B(2,1)= 0.08333333	C(2,1)= 0.08333333
A(2,2)= 0.11111111	B(2,2)= -0.02777778	C(2,2)= -0.02777778

E. Table of Atomic Basis Sets Useful in Molecular Calculations

Table of Contents

Atomic Number	Atom	Page	Atomic Number	Atom	Page	Atomic Number	Atom	Page
1	H(2S)M	78	8	O(3P)A	90	18	AR(1S)M	105
2	HE(1S)A	78	8	O(3P)N	90	19	K(2S)N	105
2	HE(1S)N	78	8	O(3P)M	91	19	K(2S)M	106
2	HE(1S)M	78	8	O(1D)A	91	20	CA(1S)N	106
2	HE(1S)S	79	8	O(1D)N	91	20	CA(1S)M	107
3	LI(2S)A	79	8	O(1D)M	92	21	SC(2D)N	107
3	LI(2S)N	79	8	O(1S)A	92	21	SC(2D)M	108
3	LI(2S)M	80	8	O(1S)N	92	22	TI(3F)N	108
3	LI(2S)S	80	8	O(1S)M	93	22	TI(3F)M	109
3	LI+(1S)A	80	8	O-(1S)N	93	23	V(4F)N	109
3	LI+(1S)N	81	9	F(2P)A	93	23	V(4F)M	110
3	LI+(1S)M	81	9	F(2P)N	94	24	CR(5D)N	110
3	LI+(1S)S	81	9	F(2P)M	94	24	CR(5D)M	111
4	BE(1S)A	82	9	F-(1S)A	94	25	MN(6S)N	111
4	BE(1S)N	82	9	F-(1S)N	95	25	MN(6S)M	112
4	BE(1S)M	82	9	F-(1S)M	95	26	FE(5D)N	112
4	BE+(1S)S	83	10	NE(1S)A	95	26	FE(5D)M	113
5	B(2P)A	83	10	NE(1S)N	96	27	CO(4F)N	113
5	B(2P)N	83	10	NE(1S)M	96	27	CO(4F)M	114
5	B(2P)M	84	11	NA(2S)N	96	28	NI(3F)N	114
6	C(3P)A	84	11	NA(2S)M	97	28	NI(3F)M	115
6	C(3P)N	84	11	NA+(1S)A	97	29	CU(2D)N	115
6	C(3P)M	85	11	NA+(1S)N	97	29	CU(2D)M	116
6	C(1D)A	85	11	NA+(1S)M	98	30	ZN(1S)N	116
6	C(1D)N	85	12	MG(1S)N	98	30	ZN(1S)M	117
6	C(1D)M	86	12	MG(1S)M	98	31	GA(2P)N	117
6	C(1S)A	86	13	AL(2P)N	99	31	GA(2P)M	118
6	C(1S)N	86	13	AL(2P)M	99	32	GE(3P)N	118
6	C(1S)M	87	14	SI(3P)N	100	32	GE(3P)M	119
7	N(4S)A	87	14	SI(3P)M	100	33	AS(4S)N	119
7	N(4S)N	87	15	P(4S)N	101	33	AS(4S)M	120
7	N(4S)M	88	15	P(4S)M	101	34	SE(3P)N	120
7	N(2D)A	88	16	S(3P)N	102	34	SE(3P)M	121
7	N(2D)N	88	16	S(3P)M	102	35	BR(2P)N	121
7	N(2D)M	89	17	CL(2P)N	103	35	BR(2P)M	122
7	N(2P)A	89	17	CL(2P)M	103	35	BR-(1S)N	122
7	N(2P)N	89	17	CL-(1S)N	104	36	KR(1S)N	123
7	N(2P)M	90	18	AR(1S)N	104	36	KR(1S)M	123

Basis Set Code

M	Minimal:	1 basis function/occupied orbital
N	Nominal:	2-3 basis functions/occupied orbital
A	Accurate:	$2\frac{1}{2}$ -4 basis functions/occupied orbital
S	Special	

ATOM=H(2S)M
TOTAL ENERGY= -0.50000

ATOMIC NUMBER= 1

BASIS SET (1,0,0)

N	L	ZETA
1	0	1.00000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SH
0.0
1.00000

ATOM=HE(1S)A
TOTAL ENERGY= -2.86168

ATOMIC NUMBER= 2

BASIS SET (3,0,0)

N	L	ZETA
1	0	1.45000
2	0	2.64100
2	0	1.72300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SHE
-0.91795
1.36211
-0.10724
-0.28189

ATOM=HE(1S)N
TOTAL ENERGY= -2.86167

ATOMIC NUMBER= 2

BASIS SET (2,0,0)

N	L	ZETA
1	0	2.90600
1	0	1.45300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SHE
-0.91793
0.18159
0.84289

ATOM=HE(1S)M
TOTAL ENERGY= -2.84766

ATOMIC NUMBER= 2

BASIS SET (1,0,0)

N	L	ZETA
1	0	1.68750

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SHE
-0.89648
1.00000

ATOM=HE(1S)S

TOTAL ENERGY= -2.86168

ATOMIC NUMBER= 2

BASIS SET (4,0,0)

N	L	ZETA
1	0	2.90600
1	0	1.45300
3	0	1.06000
2	0	0.61500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SHE

0.0

0.18179
0.84238
-0.00117
0.00222

ATOM=LI(2S)A

TOTAL ENERGY= -7.43273

ATOMIC NUMBER= 3

BASIS SET (5,0,0)

N	L	ZETA
1	0	4.69900
1	0	2.47800
2	0	1.77000
2	0	0.81000
2	0	0.64300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI

2SLI

-2.47740

-0.19632

0.11127 -0.01594
0.89726 -0.14427
0.00821 -0.08007
-0.00065 0.24522
0.00089 0.81717

ATOM=LI(2S)N

TOTAL ENERGY= -7.43272

ATOMIC NUMBER= 3

BASIS SET (4,0,0)

N	L	ZETA
1	0	4.69000
1	0	2.48300
1	0	1.64800
2	0	0.67200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI

2SLI

-2.47769

-0.19632

0.11192 -0.01907
0.88200 -0.06657
0.02147 -0.12884
0.00051 1.04323

ATOM=LI(2S)M

ATOMIC NUMBER= 3

TOTAL ENERGY= -7.41848

BASIS SET (2,0,0)

N	L	ZETA
1	0	2.69100
2	0	0.64000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI	2SLI
-2.45990	-0.19488
0.99715	-0.18142
0.01666	1.01339

ATOM=LI(2S)S

ATOMIC NUMBER= 3

TOTAL ENERGY= -7.43273

BASIS SET (4,0,0)

N	L	ZETA
1	0	4.59000
1	0	2.44800
3	0	1.04800
2	0	0.60800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI	2SLI
0.0	0.0
0.12422	-0.01210
0.89044	-0.15693
0.00250	0.32770
-0.00101	0.69538

ATOM=LI+(1S)A

ATOMIC NUMBER= 3

TOTAL ENERGY= -7.23641

BASIS SET (3,0,0)

N	L	ZETA
1	0	2.40700
2	0	4.03100
2	0	2.71100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI+
-2.79236
1.24174
-0.08383
-0.17783

ATOM=LI+(1S)N
TOTAL ENERGY= -7.23641

ATOMIC NUMBER= 3

BASIS SET (2,0,0)

N	L	ZETA
1	0	4.57300
1	0	2.44800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI+
-2.79232
0.12583
0.88907

ATOM=LI+(1S)M
TOTAL ENERGY= -7.22266

ATOMIC NUMBER= 3

BASIS SET (1,0,0)

N	L	ZETA
1	0	2.68750

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI+
-2.77148
1.00000

ATOM=LI+(1S)S
TOTAL ENERGY= -7.23641

ATOMIC NUMBER= 3

BASIS SET (4,0,0)

N	L	ZETA
1	0	4.57300
1	0	2.44800
3	0	1.56000
2	0	1.05500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SLI+
0.0
0.12595
0.88810
-0.00080
0.00048

ATOM=BE(1S)A

ATOMIC NUMBER= 4

TOTAL ENERGY= -14.57302

BASIS SET (5,0,0)

N	L	ZETA
1	0	5.74800
1	0	2.94500
3	0	3.63000
2	0	1.29000
2	0	0.85400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SBE	2SBE
-4.73266	-0.30927
0.20331	-0.01969
0.89756	-0.21113
-0.11149	-0.02030
-0.00240	0.39471
0.00085	0.68045

ATOM=BE(1S)N

ATOMIC NUMBER= 4

TOTAL ENERGY= -14.57299

BASIS SET (4,0,0)

N	L	ZETA
1	0	6.22500
1	0	3.43700
3	0	1.77600
2	0	0.86900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SBE	2SBE
-4.73267	-0.30926
0.09806	-0.00855
0.91256	-0.18811
0.00150	0.26309
-0.00055	0.77745

ATOM=BE(1S)M

ATOMIC NUMBER= 4

TOTAL ENERGY= -14.55674

BASIS SET (2,0,0)

N	L	ZETA
1	0	3.68500
2	0	0.95600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SBE	2SBE
-4.71708	-0.30864
0.99758	-0.20443
0.01241	1.01824

ATOM=BE+(1S)S

ATOMIC NUMBER= 4

TOTAL ENERGY= -14.27737

BASIS SET (4,0,0)

N	L	ZETA
1	0	6.24900
1	0	3.44100
3	0	1.66900
2	0	1.05400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SBE+	2SBE+
0.0	0.0
0.09640	-0.01062
0.91405	-0.22288
0.00274	0.46453
-0.00091	0.56795

ATOM=B(2P)A

ATOMIC NUMBER= 5

TOTAL ENERGY= -24.52906

BASIS SET (5,4,0)

N	L	ZETA
1	0	7.33800
1	0	3.99600
3	0	4.79600
2	0	1.72400
2	0	1.11000
2	1	5.50900
2	1	2.15500
2	1	1.24300
2	1	0.84500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S	2S	2P
-7.69533	-0.49470	-0.30983
0.16037	-0.01013	0.0
0.90578	-0.23838	0.0
-0.07181	-0.02820	0.0
0.00071	0.46079	0.0
-0.00006	0.62604	0.0
0.0	0.0	0.00915
0.0	0.0	0.16429
0.0	0.0	0.45440
0.0	0.0	0.43686

ATOM=B(2P)N

ATOMIC NUMBER= 5

TOTAL ENERGY= -24.52902

BASIS SET (4,3,0)

N	L	ZETA
1	0	7.73200
1	0	4.41300
3	0	2.43100
2	0	1.15200
2	1	4.55800
2	1	1.75300
2	1	0.93100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S	2S	2P
-7.69537	-0.49469	-0.30995
0.08787	-0.00720	0.0
0.92037	-0.20959	0.0
0.00265	0.27991	0.0
-0.00050	0.76890	0.0
0.0	0.0	0.01837
0.0	0.0	0.34219
0.0	0.0	0.70241

ATOM=B(2P)M

ATOMIC NUMBER= 5

TOTAL ENERGY= -24.49837

BASIS SET (2,1,0)

N	L	ZETA
1	0	4.67900
2	0	1.28800
2	1	1.21100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SB	2SB	2PB
-7.67790	-0.48387	-0.30041
0.99749	-0.22439	0.0
0.01171	1.02236	0.0
0.0	0.0	1.00000

ATOM=C(3P)A

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.68862

BASIS SET (5,4,0)

N	L	ZETA
1	0	9.05500
1	0	5.02500
3	0	6.08100
2	0	2.14100
2	0	1.35400
2	1	6.82700
2	1	2.77900
2	1	1.62500
2	1	1.05400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.32550	-0.70562	-0.43333
0.12564	-0.00329	0.0
0.92517	-0.25412	0.0
-0.05410	-0.03018	0.0
0.00138	0.49258	0.0
0.00001	0.59849	0.0
0.0	0.0	0.00842
0.0	0.0	0.17442
0.0	0.0	0.45191
0.0	0.0	0.43645

ATOM=C(3P)N

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.68855

BASIS SET (4,3,0)

N	L	ZETA
1	0	9.15300
1	0	5.38200
3	0	3.07600
2	0	1.42800
2	1	5.15200
2	1	2.17700
2	1	1.15000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.32541	-0.70553	-0.43328
0.08367	-0.00604	0.0
0.92300	-0.22226	0.0
0.00373	0.28311	0.0
-0.00049	0.77062	0.0
0.0	0.0	0.02472
0.0	0.0	0.39516
0.0	0.0	0.64975

ATOM=C(3P)M

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.62239

BASIS SET (2,1,0)

N	L	ZETA
1	0	5.67300
2	0	1.60800
2	1	1.56800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.30163	-0.67751	-0.40169
0.99744	-0.23500	0.0
0.01146	1.02468	0.0
0.0	0.0	1.00000

ATOM=C(1D)A

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.63133

BASIS SET (5,4,0)

N	L	ZETA
1	0	9.12200
1	0	5.02300
3	0	6.10300
2	0	2.12800
2	0	1.35200
2	1	6.85800
2	1	2.75800
2	1	1.59100
2	1	0.99100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.35150	-0.71868	-0.38135
0.12269	-0.00333	0.0
0.92975	-0.25546	0.0
-0.05602	-0.03012	0.0
0.00108	0.51080	0.0
0.00011	0.58028	0.0
0.0	0.0	0.00792
0.0	0.0	0.18740
0.0	0.0	0.44628
0.0	0.0	0.43929

ATOM=C(1D)N

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.63125

BASIS SET (4,3,0)

N	L	ZETA
1	0	9.17400
1	0	5.38500
3	0	3.07300
2	0	1.43300
2	1	4.85200
2	1	2.12500
2	1	1.08200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.35133	-0.71854	-0.38125
0.08261	-0.00596	0.0
0.92403	-0.22338	0.0
0.00371	0.28791	0.0
-0.00051	0.76585	0.0
0.0	0.0	0.02968
0.0	0.0	0.41704
0.0	0.0	0.63227

ATOM=C(1D)M

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.55692

BASIS SET (2,1,0)

N	L	ZETA
1	0	5.67300
2	0	1.61400
2	1	1.53600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.32641	-0.68707	-0.34004
0.99745	-0.23631	0.0
0.01134	1.02499	0.0
0.0	0.0	1.00000

ATOM=C(1S)A

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.54961

BASIS SET (5,4,0)

N	L	ZETA
1	0	9.11100
1	0	4.99500
3	0	6.08300
2	0	2.11000
2	0	1.34900
2	1	7.01000
2	1	2.78900
2	1	1.59300
2	1	0.90800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.39157	-0.73966	-0.31005
0.12590	-0.00392	0.0
0.93038	-0.25819	0.0
-0.06061	-0.02928	0.0
0.00055	0.54019	0.0
0.00031	0.55148	0.0
0.0	0.0	0.00684
0.0	0.0	0.18522
0.0	0.0	0.43764
0.0	0.0	0.46722

ATOM=C(1S)N

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.54950

BASIS SET (4,3,0)

N	L	ZETA
1	0	9.17500
1	0	5.38500
3	0	3.06900
2	0	1.44100
2	1	4.45100
2	1	2.03900
2	1	0.98000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.39141	-0.73950	-0.30993
0.08263	-0.00608	0.0
0.92409	-0.22497	0.0
0.00339	0.29534	0.0
-0.00040	0.75852	0.0
0.0	0.0	0.03949
0.0	0.0	0.44680
0.0	0.0	0.60832

ATOM=C(1S)M

ATOMIC NUMBER= 6

TOTAL ENERGY= -37.46127

BASIS SET (2,1,0)

N	L	ZETA
1	0	5.67400
2	0	1.62300
2	1	1.48700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SC	2SC	2PC
-11.36439	-0.70223	-0.25167
0.99745	-0.23826	0.0
0.01123	1.02545	0.0
0.0	0.0	1.00000

ATOM=N(4S)A

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.40093

BASIS SET (5,4,0)

N	L	ZETA
1	0	10.58600
1	0	6.03700
3	0	7.33400
2	0	2.53900
2	0	1.58800
2	1	7.67700
2	1	3.27000
2	1	1.89000
2	1	1.22200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.62898	-0.94528	-0.56754
0.11013	0.00147	0.0
0.92881	-0.26466	0.0
-0.04061	-0.03027	0.0
0.00252	0.52042	0.0
-0.00021	0.57270	0.0
0.0	0.0	0.00946
0.0	0.0	0.20936
0.0	0.0	0.47990
0.0	0.0	0.37723

ATOM=N(4S)N

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.40080

BASIS SET (4,3,0)

N	L	ZETA
1	0	10.50700
1	0	6.34600
3	0	3.71500
2	0	1.69700
2	1	5.57300
2	1	2.55500
2	1	1.35200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.62888	-0.94513	-0.56743
0.08258	-0.00542	0.0
0.92299	-0.23025	0.0
0.00458	0.28707	0.0
-0.00046	0.77038	0.0
0.0	0.0	0.03500
0.0	0.0	0.43434
0.0	0.0	0.60508

ATOM=N(4S)M

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.26890

BASIS SET (2,1,0)

N	L	ZETA
1	0	6.66500
2	0	1.92400
2	1	1.91700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.59356	-0.89250	-0.50327
0.99740	-0.24185	0.0
0.01128	1.02624	0.0
0.0	0.0	1.00000

ATOM=N(2D)A

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.29617

BASIS SET (5,4,0)

N	L	ZETA
1	0	10.59500
1	0	6.02600
3	0	7.33100
2	0	2.52800
2	0	1.58600
2	1	7.69300
2	1	3.27200
2	1	1.87700
2	1	1.16800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.66638	-0.96366	-0.50864
0.11074	0.00128	0.0
0.92969	-0.26624	0.0
-0.04234	-0.03018	0.0
0.00218	0.53711	0.0
-0.00008	0.55643	0.0
0.0	0.0	0.00900
0.0	0.0	0.21458
0.0	0.0	0.46716
0.0	0.0	0.39334

ATOM=N(2D)N

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.29602

BASIS SET (4,3,0)

N	L	ZETA
1	0	10.51300
1	0	6.34700
3	0	3.71400
2	0	1.70400
2	1	5.35900
2	1	2.51600
2	1	1.28900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.66614	-0.96344	-0.50845
0.08230	-0.00535	0.0
0.92330	-0.23152	0.0
0.00441	0.29047	0.0
-0.00040	0.76701	0.0
0.0	0.0	0.03994
0.0	0.0	0.44620
0.0	0.0	0.59603

ATOM=N(2D)M

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.14853

BASIS SET (2,1,0)

N	L	ZETA
1	0	6.66600
2	0	1.93100
2	1	1.88700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.62914	-0.90579	-0.43106
0.99741	-0.24313	0.0
0.01120	1.02655	0.0
0.0	0.0	1.00000

ATOM=N(2P)A

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.22810

BASIS SET (5,4,0)

N	L	ZETA
1	0	10.59200
1	0	6.02200
3	0	7.32300
2	0	2.52700
2	0	1.58900
2	1	7.74800
2	1	3.27500
2	1	1.86500
2	1	1.13100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.69156	-0.97632	-0.47126
0.11122	0.00128	0.0
0.92968	-0.26738	0.0
-0.04289	-0.03040	0.0
0.00205	0.54317	0.0
-0.00003	0.55072	0.0
0.0	0.0	0.00856
0.0	0.0	0.21800
0.0	0.0	0.46232
0.0	0.0	0.40088

ATOM=N(2P)N

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.22794

BASIS SET (4,3,0)

N	L	ZETA
1	0	10.52300
1	0	6.34900
3	0	3.71200
2	0	1.70800
2	1	5.19900
2	1	2.48000
2	1	1.24500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.69131	-0.97610	-0.47109
0.08175	-0.00531	0.0
0.92384	-0.23230	0.0
0.00438	0.29356	0.0
-0.00042	0.76396	0.0
0.0	0.0	0.04458
0.0	0.0	0.45543
0.0	0.0	0.58768

ATOM=N(2P)M

ATOMIC NUMBER= 7

TOTAL ENERGY= -54.06933

BASIS SET (2,1,0)

N	L	ZETA
1	0	6.66600
2	0	1.93500
2	1	1.86700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SN	2SN	2PN
-15.65373	-0.91494	-0.38421
0.99742	-0.24385	0.0
0.01111	1.02674	0.0
0.0	0.0	1.00000

ATOM=O(3P)A

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.80939

BASIS SET (5,4,0)

N	L	ZETA
1	0	12.41800
1	0	6.99500
3	0	8.68100
2	0	2.92200
2	0	1.81800
2	1	8.45000
2	1	3.74400
2	1	2.12100
2	1	1.31800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS.

1SO	2SO	2PO
-20.66860	-1.24427	-0.63186
0.09361	0.00365	0.0
0.94531	-0.27357	0.0
-0.04124	-0.02871	0.0
0.00264	0.55653	0.0
-0.00011	0.53792	0.0
0.0	0.0	0.01037
0.0	0.0	0.24554
0.0	0.0	0.47981
0.0	0.0	0.35255

ATOM=O(3P)N

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.80914

BASIS SET (4,3,0)

N	L	ZETA
1	0	11.84400
1	0	7.31100
3	0	4.34900
2	0	1.97400
2	1	5.79500
2	1	2.86700
2	1	1.46900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SO	2SO	2PO
-20.66825	-1.24396	-0.63155
0.08183	-0.00478	0.0
0.92291	-0.23757	0.0
0.00517	0.29351	0.0
-0.00042	0.76667	0.0
0.0	0.0	0.05376
0.0	0.0	0.47028
0.0	0.0	0.56243

ATOM=O(3P)M

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.54036

BASIS SET (2,1,0)

N	L	ZETA
1	0	7.65800
2	0	2.24600
2	1	2.22700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S0	2S0	2P0
-20.61306	-1.15062	-0.50303
0.99738	-0.24791	0.0
0.01109	1.02767	0.0
0.0	0.0	1.00000

ATOM=O(1D)A

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.72925

BASIS SET (5,4,0)

N	L	ZETA
1	0	12.39200
1	0	6.99600
3	0	8.65000
2	0	2.92600
2	0	1.82100
2	1	8.33000
2	1	3.73700
2	1	2.11100
2	1	1.28900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S0	2S0	2P0
-20.69318	-1.25648	-0.60069
0.09437	0.00384	0.0
0.94411	-0.27455	0.0
-0.04081	-0.02934	0.0
0.00280	0.55939	0.0
-0.00019	0.53577	0.0
0.0	0.0	0.01068
0.0	0.0	0.24779
0.0	0.0	0.47652
0.0	0.0	0.35709

ATOM=O(1D)N

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.72899

BASIS SET (4,3,0)

N	L	ZETA
1	0	11.86300
1	0	7.31300
3	0	4.34800
2	0	1.97800
2	1	5.70600
2	1	2.84400
2	1	1.43800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S0	2S0	2P0
-20.69267	-1.25606	-0.60029
0.08115	-0.00467	0.0
0.92359	-0.23825	0.0
0.00513	0.29512	0.0
-0.00041	0.76505	0.0
0.0	0.0	0.05715
0.0	0.0	0.47406
0.0	0.0	0.55877

ATOM=O(10)M
TOTAL ENERGY= -74.44673

ATOMIC NUMBER= 8

BASIS SET (3,1,0)

N	L	ZETA
1	0	7.65800
3	0	2.00000
2	0	0.25000
2	1	2.21200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

	1S0	2S0	2P0
TOTAL ENERGY	-20.63753	-1.15960	-0.46287
	0.99739	-0.24854	0.0
	0.01102	1.02784	0.0
	0.0	0.0	0.0
	0.0	0.0	1.00000

ATOM=O(11)A

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.61101

BASIS SET (5,4,0)

N	L	ZETA
1	0	12.40500
1	0	6.99800
3	0	8.65600
2	0	2.91900
2	0	1.82100
2	1	8.49700
2	1	3.74800
2	1	2.08800
2	1	1.24400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

	1S0	2S0	2P0
TOTAL ENERGY	-20.73020	-1.27510	-0.55549
	0.09384	0.00391	0.0
	0.94466	-0.27557	0.0
	-0.04080	-0.02959	0.0
	0.00266	0.56965	0.0
	-0.00014	0.52560	0.0
	0.0	0.0	0.00975
	0.0	0.0	0.25159
	0.0	0.0	0.47725
	0.0	0.0	0.35927

ATOM=O(11)N

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.61072

BASIS SET (4,3,0)

N	L	ZETA
1	0	11.88400
1	0	7.31600
3	0	4.34600
2	0	1.98300
2	1	5.51200
2	1	2.78700
2	1	1.38600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

	1S0	2S0	2P0
TOTAL ENERGY	-20.72972	-1.27473	-0.55514
	0.08027	-0.00456	0.0
	0.92445	-0.23917	0.0
	0.00510	0.29833	0.0
	-0.00042	0.76189	0.0
	0.0	0.0	0.06577
	0.0	0.0	0.48209
	0.0	0.0	0.54780

ATOM=O(1S)M

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.30740

BASIS SET (2,1,0)

N	L	ZETA
1	0	7.65900
2	0	2.25500
2	1	2.19100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S0	2S0	2P0
-20.67207	-1.17239	-0.40298
0.99740	-0.24932	0.0
0.01096	1.02803	0.0
0.0	0.0	1.00000

ATOM=O-(1S)N

ATOMIC NUMBER= 8

TOTAL ENERGY= -74.78851

BASIS SET (4,3,0)

N	L	ZETA
1	0	11.99600
1	0	7.32600
3	0	4.32400
2	0	1.82400
2	1	4.61800
2	1	2.26400
2	1	0.99400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1S0-	2S0-	2P0-
0.0	0.0	0.0
0.07660	-0.00841	0.0
0.92790	-0.22281	0.0
0.00557	0.34067	0.0
-0.00038	0.72898	0.0
0.0	0.0	0.13091
0.0	0.0	0.56376
0.0	0.0	0.44284

ATOM=F(2P)A

ATOMIC NUMBER= 9

TOTAL ENERGY= -99.40933

BASIS SET (5,4,0)

N	L	ZETA
1	0	14.20100
1	0	7.93800
3	0	9.96200
2	0	3.33200
2	0	2.05700
2	1	9.43500
2	1	4.24900
2	1	2.35600
2	1	1.43400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF	2SF	2PF
-26.38265	-1.57245	-0.72994
0.08419	0.00519	0.0
0.95503	-0.28031	0.0
-0.04226	-0.02805	0.0
0.00301	0.56794	0.0
-0.00013	0.52863	0.0
0.0	0.0	0.01055
0.0	0.0	0.26789
0.0	0.0	0.49083
0.0	0.0	0.32561

ATOM=F(2P)N

ATOMIC NUMBER= 9

TOTAL ENERGY= -99.40893

BASIS SET (4,3,0)

N	L	ZETA
1	0	13.19800
1	0	8.27800
3	0	4.98200
2	0	2.24600
2	1	6.16500
2	1	3.17600
2	1	1.61200

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF	2SF	2PF
-26.38217	-1.57205	-0.72953
0.08056	-0.00411	0.0
0.92348	-0.24286	0.0
0.00580	0.29770	0.0
-0.00044	0.76464	0.0
0.0	0.0	0.07255
0.0	0.0	0.48890
0.0	0.0	0.53155

ATOM=F(2P)M

ATOMIC NUMBER= 9

TOTAL ENERGY= -98.94211

BASIS SET (2,1,0)

N	L	ZETA
1	0	8.65000
2	0	2.56400
2	1	2.55000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF	2SF	2PF
-26.30276	-1.43061	-0.52635
0.99737	-0.25204	0.0
0.01097	1.02866	0.0
0.0	0.0	1.00000

ATOM=F-(1S)A

ATOMIC NUMBER= 9

TOTAL ENERGY= -99.45938

BASIS SET (5,4,0)

N	L	ZETA
1	0	14.09000
1	0	7.92100
3	0	9.93900
2	0	3.23000
2	0	1.83400
2	1	7.79800
2	1	3.78900
2	1	1.94600
2	1	0.96800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF-	2SF-	2PF-
-25.82946	-1.07442	-0.18083
0.08758	0.00477	0.0
0.95234	-0.27319	0.0
-0.04291	-0.02475	0.0
0.00277	0.63817	0.0
0.00006	0.46647	0.0
0.0	0.0	0.02251
0.0	0.0	0.33564
0.0	0.0	0.51644
0.0	0.0	0.26694

ATOM=F-(1S)N

ATOMIC NUMBER= 9

TOTAL ENERGY= -99.45785

BASIS SET (4,3,0)

N	L	ZETA
1	0	13.22000
1	0	8.28200
3	0	4.95200
2	0	2.09400
2	1	5.21900
2	1	2.59900
-2	1	1.15400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF	2SF	2PF
-25.82687	-1.07236	-0.17886
0.07956	-0.00824	0.0
0.92438	-0.22858	0.0
0.00594	0.33891	0.0
-0.00032	0.73161	0.0
0.0	0.0	0.14234
0.0	0.0	0.56283
0.0	0.0	0.43109

ATOM=F-(1S)M

ATOMIC NUMBER= 9

TOTAL ENERGY= -98.69651

BASIS SET (2,1,0)

N	L	ZETA
1	0	8.65800
2	0	2.49300
2	1	2.34400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SF-	2SF-	2PF-
-25.69299	-0.83397	0.14555
0.99753	-0.24039	0.0
0.01079	1.02603	0.0
0.0	0.0	1.00000

ATOM=NE(1S)A

ATOMIC NUMBER= 10

TOTAL ENERGY= -128.54710

BASIS SET (5,4,0)

N	L	ZETA
1	0	15.43900
1	0	8.80600
3	0	10.99500
2	0	3.76400
2	0	2.30100
2	1	10.54200
2	1	4.95600
2	1	2.79300
2	1	1.62300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNE	2SNE	2PNE
-32.77233	-1.93031	-0.85034
0.09218	0.00645	0.0
0.94891	-0.28821	0.0
-0.04499	-0.02632	0.0
0.00308	0.56972	0.0
-0.00003	0.53066	0.0
0.0	0.0	0.00930
0.0	0.0	0.24154
0.0	0.0	0.48233
0.0	0.0	0.36532

ATOM=NE(1S)IN

ATOMIC NUMBER= 10

TOTAL ENERGY= -128.54650

BASIS SET (4,3,0)

N	L	ZETA
1	0	14.31900
1	0	9.22400
3	0	5.61900
2	0	2.51800
2	1	6.62000
2	1	3.48400
2	1	1.76600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNE	2SNE	2PNE
-32.77162	-1.92975	-0.84974
0.08650	-0.00431	0.0
0.91716	-0.24635	0.0
0.00595	0.29901	0.0
-0.00029	0.76514	0.0
0.0	0.0	0.08944
0.0	0.0	0.50024
0.0	0.0	0.50722

ATOM=NE(1S)IN

ATOMIC NUMBER= 10

TOTAL ENERGY= -127.81220

BASIS SET (2,1,0)

N	L	ZETA
1	0	9.64200
2	0	2.87900
2	1	2.87900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNE	2SNE	2PNE
-32.66298	-1.73276	-0.56199
0.99735	-0.25495	0.0
0.01091	1.02937	0.0
0.0	0.0	1.00000

ATOM=NA(2S)IN

ATOMIC NUMBER= 11

TOTAL ENERGY= -161.85852

BASIS SET (6,3,0)

N	L	ZETA
1	0	13.11900
2	0	11.25900
3	0	6.43900
2	0	3.04000
3	0	1.24000
3	0	0.75000
2	1	7.71800
2	1	4.17100
2	1	2.27100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNA	2SNA	3SNA	2PNA
-40.47783	-2.79656	-0.18200	-1.51766
0.73943	-0.18070	0.02716	0.0
0.30385	-0.10452	0.01662	0.0
0.00726	0.22666	-0.03301	0.0
-0.00070	0.83248	-0.14463	0.0
0.00029	0.01076	0.27648	0.0
-0.00016	-0.00406	0.77807	0.0
0.0	0.0	0.0	0.07348
0.0	0.0	0.0	0.47146
0.0	0.0	0.0	0.53333

ATOM=NA(2S)M

ATOMIC NUMBER= 11

TOTAL ENERGY= -161.12392

BASIS SET (3,1,0)

N	L	ZETA
1	0	10.62590
2	0	3.28570
3	0	0.83580
2	1	3.40090

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNA	2SNA	3SNA	2PNA
0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0
0.0	1.00000	0.0	0.0
0.0	0.0	1.00000	0.0
0.0	0.0	0.0	1.00000

ATOM=NA+(1S)A

ATOMIC NUMBER= 11

TOTAL ENERGY= -161.67700

BASIS SET (5,4,0)

N	L	ZETA
1	0	15.94900
1	0	9.43900
3	0	11.62400
2	0	4.38400
2	0	2.81100
2	1	12.04800
2	1	5.70300
2	1	3.33600
2	1	2.14600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNA+	2SNA+	2PNA+
-40.75972	-3.07368	-1.79719
0.13371	0.00581	0.0
0.91835	-0.30875	0.0
-0.05827	-0.02404	0.0
0.00156	0.49163	0.0
0.00060	0.61232	0.0
0.0	0.0	0.00784
0.0	0.0	0.23017
0.0	0.0	0.45558
0.0	0.0	0.38418

ATOM=NA+(1S)N

ATOMIC NUMBER= 11

TOTAL ENERGY= -161.67660

BASIS SET (4,3,0)

N	L	ZETA
1	0	15.31400
1	0	10.15700
3	0	6.25400
2	0	2.96600
2	1	8.00000
2	1	4.31600
2	1	2.32500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNA+	2SNA+	2PNA+
-40.75946	-3.07347	-1.79697
0.09647	-0.00001	0.0
0.90707	-0.26474	0.0
0.00573	0.26942	0.0
-0.00031	0.79097	0.0
0.0	0.0	0.06123
0.0	0.0	0.45069
0.0	0.0	0.56481

ATOM=NA+(1S)M

ATOMIC NUMBER= 11

TOTAL ENERGY= -160.94800

BASIS SET (2,1,0)

N	L	ZETA
1	0	10.62600
2	0	3.28100
2	1	3.40300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNA+	2SNA+	2PNA+
-40.65887	-2.89334	-1.52886
0.99725	-0.26883	0.0
0.01077	1.03279	0.0
0.0	0.0	1.00000

ATOM=Mg(1S)M

ATOMIC NUMBER= 12

TOTAL ENERGY= -199.61429

BASIS SET (6,3,0)

N	L	ZETA
1	0	14.16100
2	0	12.22800
3	0	7.09100
2	0	3.49900
3	0	1.45800
3	0	0.89100
2	1	8.52700
2	1	4.70500
2	1	2.71900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SMG	2SMG	3SMG	2PMG
-49.03124	-3.76749	-0.25294	-2.28200
0.75305	-0.19029	0.03661	0.0
0.28823	-0.10998	0.02319	0.0
0.00660	0.20253	-0.03289	0.0
-0.00057	0.85748	-0.20290	0.0
0.00022	0.00764	0.47680	0.0
-0.00012	-0.00293	0.60001	0.0
0.0	0.0	0.0	0.07327
0.0	0.0	0.0	0.46551
0.0	0.0	0.0	0.52819

ATOM=Mg(1S)M

ATOMIC NUMBER= 12

TOTAL ENERGY= -198.85779

BASIS SET (3,1,0)

N	L	ZETA
1	0	11.60890
2	0	3.69600
3	0	1.10250
2	1	3.91290

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SMG	2SMG	3SMG	2PMG
0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0
0.0	1.00000	0.0	0.0
0.0	0.0	1.00000	0.0
0.0	0.0	0.0	1.00000

ATOM=AL (2P 1M)

ATOMIC NUMBER= 13

TOTAL ENERGY= -241.87652

BASIS SET (6,5,0)

N	L	ZETA
1	0	15.14200
2	0	13.15300
3	0	7.70700
2	0	3.95700
3	0	1.71800
3	0	1.07500
2	1	10.26000
2	1	5.72900
2	1	3.32900
3	1	1.45700
3	1	0.83800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SAL	2SAL	3SAL	2PAL	3PAL
-58.50094	-4.91069	-0.39335	-3.21835	-0.20998
0.76951	-0.19997	0.04607	0.0	0.0
0.26954	-0.11347	0.02987	0.0	0.0
0.00563	0.18565	-0.02895	0.0	0.0
-0.00033	0.87610	-0.26297	0.0	0.0
0.00013	0.00623	0.59720	0.0	0.0
-0.00007	-0.00205	0.49002	0.0	0.0
0.0	0.0	0.0	0.04275	-0.00768
0.0	0.0	0.0	0.39402	-0.07102
0.0	0.0	0.0	0.61754	-0.11313
0.0	0.0	0.0	0.00711	0.43431
0.0	0.0	0.0	-0.00149	0.64333

ATOM=AL (2P 1M)

ATOMIC NUMBER= 13

TOTAL ENERGY= -241.15376

BASIS SET (3,2,0)

N	L	ZETA
1	0	12.59100
2	0	4.10680
3	0	1.37240
2	1	4.48170
3	1	1.35520

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SAL	2SAL	3SAL	2PAL	3PAL
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=SI(3P)N

ATOMIC NUMBER= 14

TOTAL ENERGY= -288.85416

BASIS SET (6,5,0)

N	L	ZETA
1	0	16.10200
2	0	14.05700
3	0	8.30300
2	0	4.41200
3	0	2.01200
3	0	1.26500
2	1	11.34700
2	1	6.41600
2	1	3.82200
3	1	1.74300
3	1	1.02300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SSI	2SSI	3SSI	2PSI	3PSI
-68.81240	-6.15659	-0.53976	-4.25615	-0.29711
0.78563	-0.20903	0.05339	0.0	0.0
0.25127	-0.11606	0.03552	0.0	0.0
0.00457	0.17410	-0.02026	0.0	0.0
-0.00002	0.89006	-0.31394	0.0	0.0
0.00001	0.00550	0.62877	0.0	0.0
-0.00001	-0.00131	0.47043	0.0	0.0
0.0	0.0	0.0	0.03740	-0.00793
0.0	0.0	0.0	0.37241	-0.07901
0.0	0.0	0.0	0.63795	-0.14203
0.0	0.0	0.0	0.00699	0.49689
0.0	0.0	0.0	-0.00123	0.58626

ATOM=SI(3P)M

ATOMIC NUMBER= 14

TOTAL ENERGY= -288.08997

BASIS SET (3,2,0)

N	L	ZETA
1	0	13.57450
2	0	4.51000
3	0	1.63440
2	1	4.97250
3	1	1.42840

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SSI	2SSI	3SSI	2PSI	3PSI
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=P(4S)N

ATOMIC NUMBER= 15

TOTAL ENERGY= -340.71853

BASIS SET (6,5,0)

N	L	ZETA
1	0	16.81700
2	0	14.74800
3	0	8.97500
2	0	4.88400
3	0	2.30400
3	0	1.45300
2	1	12.42900
2	1	7.10700
2	1	4.31700
3	1	2.02600
3	1	1.19900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SP	2SP	3SP	2PP	3PP
-79.96941	-7.51102	-0.69627	-5.40094	-0.39164
0.81748	-0.22193	0.06076	0.0	0.0
0.21547	-0.11593	0.04002	0.0	0.0
0.00186	0.15585	-0.00865	0.0	0.0
0.00130	0.91277	-0.35946	0.0	0.0
-0.00031	0.00623	0.64031	0.0	0.0
0.00015	-0.00117	0.46938	0.0	0.0
0.0	0.0	0.0	0.03313	-0.00778
0.0	0.0	0.0	0.35164	-0.08192
0.0	0.0	0.0	0.65769	-0.16605
0.0	0.0	0.0	0.00733	0.53317
0.0	0.0	0.0	-0.00148	0.55527

ATOM=P(4S)M

ATOMIC NUMBER= 15

TOTAL ENERGY= -339.90989

BASIS SET (3,2,0)

N	L	ZETA
1	0	14.55780
2	0	4.91250
3	0	1.88060
2	1	5.48060
3	1	1.62880

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SP	2SP	3SP	2PP	3PP
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=S(3P)M

ATOMIC NUMBER= 16

TOTAL ENERGY= -397.50454

BASIS SET (6,5,0)

N	L	ZETA
1	0	17.60000
2	0	15.45000
3	0	9.68100
2	0	5.36200
3	0	2.58700
3	0	1.63000
2	1	13.41900
2	1	7.75200
2	1	4.79900
3	1	2.32400
3	1	1.31800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SS	2SS	3SS	2PS	3PS
-92.00397	-9.00419	-0.87935	-6.68249	-0.43726
0.84227	-0.23262	0.06730	0.0	0.0
0.18755	-0.11806	0.04501	0.0	0.0
-0.00026	0.13628	0.00409	0.0	0.0
0.00234	0.93755	-0.40244	0.0	0.0
-0.00055	0.00710	0.66007	0.0	0.0
0.00026	-0.00108	0.45968	0.0	0.0
0.0	0.0	0.0	0.03095	-0.00773
0.0	0.0	0.0	0.33759	-0.08288
0.0	0.0	0.0	0.66960	-0.18488
0.0	0.0	0.0	-0.00768	0.55745
0.0	0.0	0.0	-0.00082	0.54591

ATOM=S(3P)M

ATOMIC NUMBER= 16

TOTAL ENERGY= -396.62761

BASIS SET (3,2,0)

N	L	ZETA
1	0	15.54090
2	0	5.31440
3	0	2.12230
2	1	5.98850
3	1	1.82730

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SS	2SS	3SS	2PS	3PS
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=CL (2P)M

ATOMIC NUMBER= 17

TOTAL ENERGY= -459.48160

BASIS SET (6,5,0)

N	L	ZETA
1	0	18.41600
2	0	16.13600
3	0	10.38800
2	0	5.83900
3	0	2.87300
3	0	1.80900
2	1	14.45800
2	1	8.45500
2	1	5.29800
3	1	2.60900
3	1	1.45600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCL	2SCL	3SCL	2PCL	3PCL
-104.88373	-10.60727	-1.07266	-8.07209	-0.50621
0.86287	-0.24191	0.07295	0.0	0.0
0.16436	-0.12093	0.04999	0.0	0.0
-0.00209	0.12045	0.01589	0.0	0.0
0.00323	0.95889	-0.43999	0.0	0.0
-0.00073	0.00829	0.66751	0.0	0.0
0.00034	-0.00113	0.46110	0.0	0.0
0.0	0.0	0.0	0.02803	-0.00732
0.0	0.0	0.0	0.31782	-0.08129
0.0	0.0	0.0	0.68823	-0.20352
0.0	0.0	0.0	0.00893	0.57531
0.0	0.0	0.0	-0.00060	0.53643

ATOM=CL (2P)M

ATOMIC NUMBER= 17

TOTAL ENERGY= -458.52370

BASIS SET (3,2,0)

N	L	ZETA
1	0	16.52390
2	0	5.71520
3	0	2.35610
2	1	6.49660
3	1	2.03870

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCL	2SCL	3SCL	2PCL	3PCL
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=CL-(1S)N

ATOMIC NUMBER= 17

TOTAL ENERGY= -459.57360

BASIS SET (6,4,0)

N	L	ZETA
1	0	18.57500
2	0	16.32900
3	0	10.21700
2	0	5.79800
3	0	2.82300
3	0	1.65100
2	1	10.20300
2	1	5.58500
3	1	2.49700
3	1	1.22400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCL-	2SCL-	3SCL-	2PCL-	3PCL-
-104.50086	-10.22595	-0.73031	-7.69225	-0.14772
0.85189	-0.23882	0.07001	0.0	0.0
0.17649	-0.11908	0.04802	0.0	0.0
-0.00074	0.14005	0.01033	0.0	0.0
0.00245	0.93670	-0.42149	0.0	0.0
-0.00052	0.00654	0.70660	0.0	0.0
0.00021	-0.00035	0.43162	0.0	0.0
0.0	0.0	0.0	0.21126	-0.05028
0.0	0.0	0.0	0.81783	-0.21340
0.0	0.0	0.0	0.01585	0.61008
0.0	0.0	0.0	-0.00394	0.52453

ATOM=AR(1S)N

ATOMIC NUMBER= 18

TOTAL ENERGY= -526.81693

BASIS SET (6,5,0)

N	L	ZETA
1	0	19.25000
2	0	16.78100
3	0	11.19100
2	0	6.33200
3	0	3.14300
3	0	1.98000
2	1	15.31700
2	1	9.05300
2	1	5.77000
3	1	2.89300
3	1	1.60500

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SAR	2SAR	3SAR	2PAR	3PAR
-118.60946	-12.32176	-1.27695	-9.57115	-0.59066
0.88067	-0.25013	0.07796	0.0	0.0
0.14447	-0.12632	0.05512	0.0	0.0
-0.00394	0.09909	0.02585	0.0	0.0
0.00406	0.98695	-0.47093	0.0	0.0
-0.00089	0.01026	0.67724	0.0	0.0
0.00040	-0.00152	0.45728	0.0	0.0
0.0	0.0	0.0	0.02782	-0.00748
0.0	0.0	0.0	0.30978	-0.08078
0.0	0.0	0.0	0.69415	-0.21613
0.0	0.0	0.0	0.00807	0.58674
0.0	0.0	0.0	-0.00137	0.53086

ATOM=AR(15)M
TOTAL ENERGY= -525.76526

ATOMIC NUMBER= 18

BASIS SET (3,2,0)

N	L	ZETA
1	0	17.50750
2	0	6.11520
3	0	2.58560
2	1	7.00410
3	1	2.25470

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SAR	2SAR	3SAR	2PAR	3PAR
0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	1.00000

ATOM=K(12S)M
TOTAL ENERGY= -599.16424

ATOMIC NUMBER= 19

BASIS SET (8,5,0)

N	L	ZETA
1	0	20.14300
2	0	17.43500
3	0	12.13600
2	0	6.84900
3	0	3.42200
3	0	2.28200
4	0	1.19200
4	0	0.72300
2	1	16.00000
2	1	9.62900
2	1	6.24600
3	1	3.23200
3	1	1.92600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SK	2SK	3SK	4SK	2PK	3PK
-133.53243	-14.48985	-1.74867	-0.14737	-11.51923	-0.95433
0.89324	-0.25667	0.08446	-0.01631	0.0	0.0
0.13077	-0.13524	0.06256	-0.01277	0.0	0.0
-0.00615	0.07220	0.03645	-0.01038	0.0	0.0
-0.00519	1.02143	-0.51273	0.10643	0.0	0.0
-0.00147	0.01442	0.68327	-0.16450	0.0	0.0
-0.00089	-0.00394	0.45044	-0.06836	0.0	0.0
-0.00026	0.00088	-0.00074	0.42326	0.0	0.0
0.00012	-0.00039	0.00089	0.65782	0.0	0.0
0.0	0.0	0.0	0.0	0.02900	-0.00881
0.0	0.0	0.0	0.0	0.30104	-0.08186
0.0	0.0	0.0	0.0	0.69901	-0.24436
0.0	0.0	0.0	0.0	0.00867	0.58915
0.0	0.0	0.0	0.0	-0.00160	0.52260

ATOM=K(2S)M

ATOMIC NUMBER= 19

TOTAL ENERGY= -598.08989

BASIS SET (4,2,0)

N	L	ZETA
1	0	18.48950
2	0	6.50310
3	0	2.89330
4	0	0.87380
2	1	7.51360
3	1	2.57520

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SK	2SK	3SK	4SK	2PK	3PK
0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=CA(1S)N

ATOMIC NUMBER= 20

TOTAL ENERGY= -676.75760

BASIS SET (8,5,0)

N	L	ZETA
1	0	21.12500
2	0	18.25300
3	0	12.86700
2	0	7.33200
3	0	3.67400
3	0	2.54500
4	0	1.45500
4	0	0.87500
2	1	17.00000
2	1	10.23200
2	1	6.71500
3	1	3.52700
3	1	2.20300

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCA	2SCA	3SCA	4SCA	2PCA	3PCA
-149.36309	-16.82258	-2.24517	-0.19541	-13.62917	-1.34051
0.89911	-0.26108	0.08990	-0.02146	0.0	0.0
0.12409	-0.14105	0.06960	-0.01756	0.0	0.0
-0.00688	0.06099	0.04659	-0.01472	0.0	0.0
0.00559	1.03780	-0.55278	0.14093	0.0	0.0
-0.00177	0.01623	0.72517	-0.21081	0.0	0.0
0.00118	-0.00531	0.41276	-0.09695	0.0	0.0
-0.00034	0.00110	-0.00238	0.50157	0.0	0.0
0.00014	-0.00042	0.00081	0.60261	0.0	0.0
0.0	0.0	0.0	0.0	0.02750	-0.00898
0.0	0.0	0.0	0.0	0.29673	-0.08393
0.0	0.0	0.0	0.0	0.70286	-0.26706
0.0	0.0	0.0	0.0	0.00870	0.61542
0.0	0.0	0.0	0.0	-0.00175	0.49520

ATOM=CA(1S)M

ATOMIC NUMBER= 20

TOTAL ENERGY= -675.63389

BASIS SET (4,2,0)

N	L	ZETA
1	0	19.47300
2	0	6.88820
3	0	3.20050
4	0	1.09950
2	1	8.02070
3	1	2.88610

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCA	2SCA	3SCA	4SCA	2PCA	3PCA
0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=SC(2D)M

ATOMIC NUMBER= 21

TOTAL ENERGY= -759.73514

BASIS SET (8,5,4)

N	L	ZETA
1	0	22.09500
2	0	19.03400
3	0	13.57900
2	0	7.80600
3	0	3.95800
3	0	2.74500
4	0	1.54700
4	0	0.92100
2	1	18.00000
2	1	10.84000
2	1	7.18700
3	1	3.81400
3	1	2.38400
3	2	8.60000
3	2	4.09200
3	2	2.16000
3	2	1.16900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SSC	2SSC	3SSC	4SSC	2PSC	3PSC	3DSC
-165.89913	-19.08028	-2.56702	-0.20993	-15.66796	-1.57425	-0.34337
0.90525	-0.26540	0.09336	-0.02216	0.0	0.0	0.0
0.11719	-0.14583	0.07499	-0.01900	0.0	0.0	0.0
-0.00776	0.05558	0.05403	-0.01768	0.0	0.0	0.0
0.00601	1.04838	-0.57892	0.14862	0.0	0.0	0.0
-0.00185	0.01687	0.72915	-0.21643	0.0	0.0	0.0
0.00120	-0.00541	0.41496	-0.08910	0.0	0.0	0.0
-0.00033	0.00109	-0.00139	0.51474	0.0	0.0	0.0
0.00014	-0.00041	0.00059	0.58983	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.02608	-0.00873	0.0
0.0	0.0	0.0	0.0	0.29251	-0.08366	0.0
0.0	0.0	0.0	0.0	0.70658	-0.27990	0.0
0.0	0.0	0.0	0.0	0.00905	0.62967	0.0
0.0	0.0	0.0	0.0	-0.00168	0.48531	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.02764
0.0	0.0	0.0	0.0	0.0	0.0	0.28726
0.0	0.0	0.0	0.0	0.0	0.0	0.53334
0.0	0.0	0.0	0.0	0.0	0.0	0.32001

ATOM=SC(2D)H

ATOMIC NUMBER= 21

TOTAL ENERGY= -758.40415

BASIS SET (4,2,1)

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS						
1SSC	2SSC	3SSC	4SSC	2PSC	3PSC	3DSC
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=TI(3F)H

ATOMIC NUMBER= 22

TOTAL ENERGY= -848.40538

BASIS SET (8,5,4)

N L		ZETA
1	0	23.09100
2	0	19.87700
3	0	14.42500
2	0	8.29100
3	0	4.19600
3	0	2.88200
4	0	1.63400
4	0	0.95800
2	1	19.00000
2	1	11.46200
3	1	7.65600
3	1	4.10100
3	1	2.55300
3	2	9.10000
3	2	4.42000
3	2	2.37000
3	2	1.31400

ATOM=TI(3F)M

ATOMIC NUMBER= 22

TOTAL ENERGY= -846.81560

BASIS SET (4,2,1)

N	L	ZETA
1	0	21.44090
2	0	7.68830
3	0	3.67770
4	0	1.20420
2	1	9.03240
3	1	3.36790
3	2	2.71380

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1STI	2STI	3STI	4STI	2PTI	3PTI	3DTI
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=V(4F)N

ATOMIC NUMBER= 23

TOTAL ENERGY= -942.88363

BASIS SET (8,5,4)

N	L	ZETA
1	0	24.07800
2	0	20.69700
3	0	15.15700
2	0	8.76200
3	0	4.49000
3	0	3.09000
4	0	1.72600
4	0	0.99800
2	1	20.00000
2	1	12.06400
2	1	8.12100
3	1	4.39100
3	1	2.72200
3	2	9.60000
3	2	4.76000
3	2	2.57500
3	2	1.43000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SV	2SV	3SV	4SV	2PV	3PV	3DV
-201.50207	-23.87437	-3.18291	-0.23039	-20.02226	-2.01894	-0.50931
0.91365	-0.27214	0.09830	-0.02235	0.0	0.0	0.0
0.10755	-0.15579	0.08328	-0.02029	0.0	0.0	0.0
-0.00818	0.04051	0.06278	-0.01955	0.0	0.0	0.0
0.00587	1.07288	-0.61182	0.15119	0.0	0.0	0.0
-0.00168	0.01816	0.74043	-0.21310	0.0	0.0	0.0
0.00105	-0.00561	0.41178	-0.07986	0.0	0.0	0.0
-0.00028	0.00110	-0.00044	0.50574	0.0	0.0	0.0
0.00011	-0.00041	0.00030	0.60228	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.02323	-0.00799	0.0
0.0	0.0	0.0	0.0	0.28672	-0.08233	0.0
0.0	0.0	0.0	0.0	0.71211	-0.29847	0.0
0.0	0.0	0.0	0.0	0.00968	0.63867	0.0
0.0	0.0	0.0	0.0	-0.00143	0.48458	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03194
0.0	0.0	0.0	0.0	0.0	0.0	0.32051
0.0	0.0	0.0	0.0	0.0	0.0	0.53683
0.0	0.0	0.0	0.0	0.0	0.0	0.26762

ATOM=V(4F)M
TOTAL ENERGY= -940.97195

ATOMIC NUMBER= 23

BASIS SET (4,2,1)

ZETA

1	0	22.42560
2	0	8.09070
3	0	3.90310
4	0	1.24530
2	1	9.53640
3	1	3.59500
3	2	2.99430

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

ATOM=CR (5D)N.

TOTAL ENERGY= -1043.30890

ATOMIC NUMBER= 24

BASIS SET (8,5,4)

ZETA
NL

1	0	25.04100
1	0	21.42400
3	0	16.48400
3	0	9.24700
3	0	4.67200
3	0	3.14400
3	0	1.86500
4	0	1.06000
4	0	21.00000
2	1	13.09500
2	1	8.66000
2	1	4.66400
3	1	2.88200
3	1	10.10000
3	2	5.08200
3	2	2.74700
3	2	1.51400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

ATOM=CR(50M)
TOTAL ENERGY= -1041.00620

ATOMIC NUMBER= 24

BASIS SET (4,2,1)

N L ZETA

1	0	23.41380
2	0	8.49190
3	0	4.12260
4	0	1.28330
2	1	10.03760
3	1	3.82200
3	2	3.25220

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCR	2SCR	3SCR	4SCR	2PCR	3PCR	3DCR
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=NN(65M)
TOTAL ENERGY= -1149.86530

ATOMIC NUMBER= 25

BASIS SET (8,5,4)

N L ZETA

1	0	26.05000
2	0	22.27300
2	0	17.25800
3	0	9.71400
3	0	4.92300
3	0	3.29000
4	0	1.92400
4	0	1.08500
2	1	22.00000
2	1	13.64300
2	1	9.14600
3	1	4.94600
3	1	3.04200
3	2	10.60000
3	2	5.40400
3	2	2.93500
3	2	1.62000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SMN	2SMN	3SMN	4SMN	2PMN	3PMN	3DMN
-240.53247	-29.10862	-3.81585	-0.24746	-24.81174	-2.47872	-0.63799
0.92141	-0.27804	0.10230	-0.02222	0.0	0.0	0.0
0.09925	-0.16596	0.08747	-0.02013	0.0	0.0	0.0
-0.00843	0.02898	0.05483	-0.01558	0.0	0.0	0.0
0.00492	1.09496	-0.61569	0.14338	0.0	0.0	0.0
-0.00134	0.01922	0.80085	-0.21565	0.0	0.0	0.0
-0.00083	-0.00618	0.35619	-0.06488	0.0	0.0	0.0
-0.00024	0.00141	-0.00503	0.47125	0.0	0.0	0.0
0.00009	-0.00049	0.00157	0.64026	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01887	-0.00668	0.0
0.0	0.0	0.0	0.0	0.25166	-0.07111	0.0
0.0	0.0	0.0	0.0	0.74771	-0.32050	0.0
0.0	0.0	0.0	0.0	0.01245	0.64370	0.0
0.0	0.0	0.0	0.0	-0.00194	0.48427	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03434
0.0	0.0	0.0	0.0	0.0	0.0	0.34059
0.0	0.0	0.0	0.0	0.0	0.0	0.53636
0.0	0.0	0.0	0.0	0.0	0.0	0.24470

ATOM=MN(6S)M

ATOMIC NUMBER= 25

TOTAL ENERGY= -1147.10670

BASIS SET (4,2,1)

N	L	ZETA
1	0	24.39570
2	0	8.89690
3	0	4.33930
4	0	1.32080
2	1	10.54200
3	1	4.03640
3	2	3.50940

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SMN	2SMN	3SMN	4SMN	2PMN	3PMN	3DMN
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=FE(5D)N

ATOMIC NUMBER= 26

TOTAL ENERGY= -1262.44250

BASIS SET (8,5,4)

N	L	ZETA
1	0	27.05400
2	0	23.14200
3	0	17.86900
2	0	10.16300
3	0	5.23800
3	0	3.51600
4	0	2.01800
4	0	1.12600
2	1	23.00000
2	1	14.21500
2	1	9.60300
3	1	5.22700
3	1	3.20600
3	2	11.10000
3	2	5.72900
3	2	3.10000
3	2	1.67700

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SFE	2SFE	3SFE	4SFE	2PFE	3PFE	3DPE
-261.37171	-31.93448	-4.16849	-0.25768	-27.41270	-2.74123	-0.64588
0.92398	-0.28035	0.10393	-0.02228	0.0	0.0	0.0
0.09604	-0.16773	0.09081	-0.02072	0.0	0.0	0.0
-0.00844	0.03100	0.05990	-0.01693	0.0	0.0	0.0
0.00503	1.09565	-0.63175	0.14586	0.0	0.0	0.0
-0.00135	0.01826	0.77334	-0.20679	0.0	0.0	0.0
0.00081	-0.00518	0.38877	-0.07173	0.0	0.0	0.0
-0.00022	0.00107	-0.00376	0.46731	0.0	0.0	0.0
0.00008	-0.00037	0.00139	0.64613	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01816	-0.00640	0.0
0.0	0.0	0.0	0.0	0.25317	-0.07163	0.0
0.0	0.0	0.0	0.0	0.74593	-0.32558	0.0
0.0	0.0	0.0	0.0	0.01265	0.64707	0.0
0.0	0.0	0.0	0.0	-0.00184	0.48370	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03494
0.0	0.0	0.0	0.0	0.0	0.0	0.34662
0.0	0.0	0.0	0.0	0.0	0.0	0.53028
0.0	0.0	0.0	0.0	0.0	0.0	0.25027

ATOM=FE(50)M

ATOMIC NUMBER= 26

TOTAL ENERGY= -1259.08550

BASIS SET (4,2,1)

	1SFE	2SFE	3SFE	4SFE	2PFE	3PFE	3DFE
N	L	ZETA					
1	0	25.38100	0.0	0.0	0.0	0.0	0.0
2	0	9.29950	0.0	0.0	0.0	0.0	0.0
3	0	4.55870	0.0	0.0	0.0	0.0	0.0
4	0	1.35850	0.0	1.00000	0.0	0.0	0.0
2	1	11.04440	0.0	0.0	1.00000	0.0	0.0
3	1	4.25930	0.0	0.0	0.0	1.00000	0.0
3	2	3.72660	0.0	0.0	0.0	0.0	1.00000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

ATOM=CO(4F)N

ATOMIC NUMBER= 27

TOTAL ENERGY= -1381.41330

BASIS SET (8,5,4)

	N	L	ZETA
1	0	28.06800	
2	0	24.02200	
3	0	18.63500	
2	0	10.64400	
3	0	5.49200	
3	0	3.67600	
4	0	2.08700	
4	0	1.15500	
2	1	24.00000	
2	1	14.77500	
2	1	10.05400	
3	1	5.50300	
3	1	3.36600	
3	2	11.60000	
3	2	6.03800	
3	2	3.25900	
3	2	1.74700	

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

	1SCO	2SCO	3SCO	4SCO	2PCO	3PCO	3DCO
-283.06375							
0.92588	-0.28237	-34.86728	-4.52330	-0.26690	-30.11912	-3.00523	-0.67437
0.09374	-0.17151		0.10530	-0.02222	0.0	0.0	0.0
-0.00844	0.02541		0.09381	-0.02112	0.0	0.0	0.0
0.00496	1.10422		0.06314	-0.01773	0.0	0.0	0.0
-0.00129	0.01962		-0.64142	0.14627	0.0	0.0	0.0
0.00077	-0.00579		0.77559	-0.20584	0.0	0.0	0.0
-0.00021	0.00122		0.38829	-0.06690	0.0	0.0	0.0
0.00008	-0.00042		-0.00345	0.47277	0.0	0.0	0.0
0.0	0.0		0.00131	0.64135	0.0	0.0	0.0
0.0	0.0		0.0	0.0	0.01748	-0.00602	0.0
0.0	0.0		0.0	0.0	0.25605	-0.07301	0.0
0.0	0.0		0.0	0.0	0.74290	-0.32882	0.0
0.0	0.0		0.0	0.0	0.01275	0.64999	0.0
0.0	0.0		0.0	0.0	-0.00172	0.48313	0.0
0.0	0.0		0.0	0.0	0.0	0.0	0.03574
0.0	0.0		0.0	0.0	0.0	0.0	0.35444
0.0	0.0		0.0	0.0	0.0	0.0	0.52547
0.0	0.0		0.0	0.0	0.0	0.0	0.24964

ATOM=CO(4F)M

ATOMIC NUMBER= 27

TOTAL ENERGY= -1377.37440

BASIS SET (4,2,1)

N	L	ZETA
1	0	26.36680
2	0	9.70250
3	0	4.77410
4	0	1.39410
2	1	11.54620
3	1	4.47820
3	2	3.95180

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

ATOM=N I (3 F) N

ATOMIC NUMBER= 28

TOTAL ENERGY= -1506.86950

BASIS SET (8,5,4)

	N	L	ZETA
1	1	0	29.07500
2	2	0	24.87700
3	3	0	19.41000
4	4	0	11.11100
5	5	0	5.75000
6	6	0	3.84300
7	7	0	2.16300
8	8	0	1.18800
9	9	0	25.00000
10	10	1	15.32800
11	11	1	10.50000
12	12	1	5.78100
13	13	1	3.52600
14	14	2	12.10000
15	15	2	6.36000
16	16	2	3.42800
17	17	2	1.82000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNI	2SNI	3SNI	4SNI	2PNI	3PNI	3DNI
-305.61712	-37.91660	-4.88663	-0.27563	-32.94051	-3.27642	-0.70566
0.92803	-0.28434	0.10657	-0.02213	0.0	0.0	0.0
0.09127	-0.17444	0.09623	0.02136	0.0	0.0	0.0
-0.00853	0.02354	0.06417	-0.01793	0.0	0.0	0.0
0.00492	1.10908	-0.64832	0.14592	0.0	0.0	0.0
-0.00125	0.02007	0.77448	-0.20354	0.0	0.0	0.0
0.00075	-0.00588	0.39106	-0.06412	0.0	0.0	0.0
-0.00019	0.00123	-0.00283	0.47193	0.0	0.0	0.0
0.00007	-0.00043	0.00114	0.64275	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01681	-0.00567	0.0
0.0	0.0	0.0	0.0	0.25990	-0.07455	0.0
0.0	0.0	0.0	0.0	0.73904	-0.33150	0.0
0.0	0.0	0.0	0.0	0.01273	0.65165	0.0
0.0	0.0	0.0	0.0	-0.00156	0.48378	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03624
0.0	0.0	0.0	0.0	0.0	0.0	0.35880
0.0	0.0	0.0	0.0	0.0	0.0	0.52279
0.0	0.0	0.0	0.0	0.0	0.0	0.25001

ATOM=NI(3F)M

ATOMIC NUMBER= 28

TOTAL ENERGY= -1502.04870

BASIS SET (4,2,1)

N L ZETA

1	0	27.35260
2	0	10.10630
3	0	4.98700
4	0	1.42770
2	1	12.04760
3	1	4.69500
3	2	4.17650

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SNI	2SNI	3SNI	4SNI	2PNI	3PNI	3DNI
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=CU(2D)N

ATOMIC NUMBER= 29

TOTAL ENERGY= -1638.94850

BASIS SET (8,5,4)

N L ZETA

1	0	30.08400
2	0	25.71600
3	0	20.24000
2	0	11.56700
3	0	5.98200
3	0	3.97700
4	0	2.22900
4	0	1.21500
2	1	26.00000
2	1	15.85900
2	1	10.94100
3	1	6.05600
3	1	3.68400
3	2	12.60000
3	2	6.68100
3	2	3.59900
3	2	1.89600

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCU	2SCU	3SCU	4SCU	2PCU	3PCU	3DCU
-329.03262	-41.08353	-5.25933	-0.28409	-35.87789	-3.55557	-0.73886
0.92989	-0.28614	0.10772	-0.02202	0.0	0.0	0.0
0.08918	-0.17692	0.09785	-0.02139	0.0	0.0	0.0
-0.00876	0.02401	0.06203	-0.01735	0.0	0.0	0.0
0.00489	1.11174	-0.65045	0.14435	0.0	0.0	0.0
-0.00122	0.01979	0.78610	-0.20431	0.0	0.0	0.0
0.00071	-0.00566	0.38070	-0.03758	0.0	0.0	0.0
-0.00019	0.00118	-0.00290	0.47560	0.0	0.0	0.0
0.00007	-0.00041	0.00111	0.63972	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01630	-0.00532	0.0
0.0	0.0	0.0	0.0	0.26513	-0.07677	0.0
0.0	0.0	0.0	0.0	0.73371	-0.33299	0.0
0.0	0.0	0.0	0.0	0.01274	0.65349	0.0
0.0	0.0	0.0	0.0	-0.00144	0.48397	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03670
0.0	0.0	0.0	0.0	0.0	0.0	0.36232
0.0	0.0	0.0	0.0	0.0	0.0	0.52013
0.0	0.0	0.0	0.0	0.0	0.0	0.25074

ATOM=CU(20JM)

ATOMIC NUMBER= 29

TOTAL ENERGY= -1633.23930

BASIS SET (4,2,1)

N	L	ZETA
1	0	28.33860
2	0	10.50990
3	0	5.19810
4	0	1.66060
2	1	12.54850
3	1	4.91020
3	2	4.40020

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SCU	2SCU	3SCU	4SCU	2PCU	3PCU	3DCU
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=ZN(15JM)

ATOMIC NUMBER= 30

TOTAL ENERGY= -1777.84640

BASIS SET (8,5,4)

N	L	ZETA
1	0	31.07000
2	0	26.49900
3	0	21.00300
2	0	12.01300
3	0	6.24000
3	0	4.13900
4	0	2.29900
4	0	1.24400
2	1	27.00000
2	1	16.42300
2	1	11.39100
3	1	6.33900
3	1	3.84200
3	2	13.10000
3	2	7.00800
3	2	3.77900
3	2	1.98100

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SZN	2SZN	3SZN	4SZN	2PZN	3PZN	3DZN
-353.30244	-44.36025	-5.63637	-0.29175	-38.92339	-3.83787	-0.78106
0.93268	-0.28816	0.10888	-0.02188	0.0	0.0	0.0
0.08602	-0.17876	0.09962	-0.02145	0.0	0.0	0.0
-0.00896	0.02785	0.06002	-0.01686	0.0	0.0	0.0
0.00486	1.11112	-0.65356	0.14294	0.0	0.0	0.0
-0.00119	0.01930	0.78438	-0.20138	0.0	0.0	0.0
0.00068	-0.00526	0.38430	-0.09537	0.0	0.0	0.0
-0.00018	0.00107	-0.00254	0.47479	0.0	0.0	0.0
0.00007	-0.00037	0.00102	0.64121	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01568	-0.00509	0.0
0.0	0.0	0.0	0.0	0.26764	-0.07716	0.0
0.0	0.0	0.0	0.0	0.73110	-0.33602	0.0
0.0	0.0	0.0	0.0	0.01296	0.65314	0.0
0.0	0.0	0.0	0.0	-0.00137	0.48665	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.03703
0.0	0.0	0.0	0.0	0.0	0.0	0.36419
0.0	0.0	0.0	0.0	0.0	0.0	0.51794
0.0	0.0	0.0	0.0	0.0	0.0	0.25179

[illegible]

ATOMIC NUMBER= 31

BASIS SET (4,3,1)

N	L	ZETA
1	0	30.30940
2	0	11.29950
3	0	5.66540
4	0	1.76670
2	1	13.54540
3	1	5.40120
4	1	1.55540
3	2	5.03110

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

ATOMIC NUMBER= 32

BASIS SET (8,7,4)

N	L	ZETA
1	0	33.07600
2	0	28.16500
3	0	22.47100
2	0	12.93300
3	0	6.71100
3	0	4.55100
4	0	2.65700
4	0	1.55200
2	1	7.23200
2	1	4.59800
2	1	2.29600
3	1	1.25400
3	1	29.00000
4	1	17.58600
4	1	12.31900
3	2	14.10000
3	2	7.79900
3	2	4.37300
3	2	2.53400

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SGE	2SGE	3SGE	4SGE	2PGE	3PGE	4PGE	3DGE
-405.24282	-52.14916	-7.18994	-0.55244	-46.23500	-5.16059	-0.28695	-1.63388
0.93634	-0.29136	0.11232	-0.02884	0.0	0.0	0.0	0.0
0.08174	-0.18315	0.10506	-0.02902	0.0	0.0	0.0	0.0
-0.00924	0.02832	0.06121	-0.02204	0.0	0.0	0.0	0.0
0.00497	1.11577	-0.67219	0.18839	0.0	0.0	0.0	0.0
-0.00131	0.02077	0.81127	-0.26579	0.0	0.0	0.0	0.0
0.00081	-0.00659	0.35933	-0.07601	0.0	0.0	0.0	0.0
-0.00023	0.00140	-0.00475	0.60405	0.0	0.0	0.0	0.0
0.00009	-0.00051	0.00173	0.51093	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01470	0.55217	-0.13541	0.0
0.0	0.0	0.0	0.0	-0.00170	0.58573	-0.10332	0.0
0.0	0.0	0.0	0.0	0.00038	0.01022	0.47872	0.0
0.0	0.0	0.0	0.0	-0.00015	-0.00174	0.63300	0.0
0.0	0.0	0.0	0.0	0.01447	-0.00593	0.00164	0.0
0.0	0.0	0.0	0.0	0.26800	-0.06831	0.00954	0.0
0.0	0.0	0.0	0.0	0.72952	-0.36353	0.07825	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.03904
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.36799
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.52983
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.19920

ATOM=AS(4S)M
TOTAL ENERGY= -22.27+1.3930

ATOMIC NUMBER= 33

BASIS SET (4,3,1)

N L ZETA

1	0	32.27830
2	0	12.06350
3	0	6.19850
4	0	2.23600
2	1	14.53680
3	1	5.94990
4	1	1.86230
3	2	5.79280

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SAS	2SAS	3SAS	4SAS	2PAS	3PAS	4PAS	3DAS
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=SE(3P)M
TOTAL ENERGY= -23.99+8.6630

ATOMIC NUMBER= 34

BASIS SET (8,7,4)

N L ZETA

1	0	35.08500
2	0	29.89100
3	0	23.98000
2	0	13.86800
3	0	7.21300
3	0	5.01700
4	0	3.08900
4	0	1.85500
2	1	31.00000
2	1	18.78900
2	1	13.28800
3	1	7.87100
3	1	5.18000
4	1	2.70200
4	1	1.49900
3	2	15.10000
3	2	8.55600
3	2	4.91600
3	2	2.96800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SSE	2SSE	3SSE	4SSE	2PSE	3PSE	4PSE	3DSE
-460.86600	-60.66795	-8.93151	-0.83678	-54.26796	-6.66095	-0.40238	-2.64903
0.93943	-0.29414	0.11579	-0.03389	0.0	0.0	0.0	0.0
0.07787	-0.18742	0.11089	-0.03495	0.0	0.0	0.0	0.0
-0.00893	0.02509	0.06644	-0.02635	0.0	0.0	0.0	0.0
-0.00475	1.12328	-0.69675	0.22214	0.0	0.0	0.0	0.0
-0.00136	0.02270	0.83136	-0.30448	0.0	0.0	0.0	0.0
0.00090	-0.00827	0.34220	-0.10603	0.0	0.0	0.0	0.0
-0.00026	0.00173	-0.00517	0.65634	0.0	0.0	0.0	0.0
0.00010	-0.00060	0.00206	0.47449	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01379	-0.00564	0.00187	0.0
0.0	0.0	0.0	0.0	0.26051	-0.06583	0.001108	0.0
0.0	0.0	0.0	0.0	0.73527	-0.37933	0.09974	0.0
0.0	0.0	0.0	0.0	0.01741	0.53119	-0.16053	0.0
0.0	0.0	0.0	0.0	-0.00301	0.60503	-0.14093	0.0
0.0	0.0	0.0	0.0	0.00059	0.01005	0.36615	0.0
0.0	0.0	0.0	0.0	-0.00024	-0.00133	0.55609	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04061
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.37293
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.55048
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.15168

ATOM=SE(3P)M
TOTAL ENERGY= -2392.72740

ATOMIC NUMBER= 34

BASIS SET (4,3,1)

N L ZETA

1	0	33.26220
2	0	12.44420
3	0	6.46780
4	0	2.43940
2	1	15.03260
3	1	6.23500
4	1	2.07180
3	2	6.15900

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SSE	2SSE	3SSE	4SSE	2PSE	3PSE	4PSE	3DSE
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.00000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.00000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.00000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.00000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.00000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.00000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.00000

ATOM=BR(2P)N
TOTAL ENERGY= -2572.44000

ATOMIC NUMBER= 35

BASIS SET (8,7,4)

N L ZETA

1	0	36.10700
2	0	30.76800
3	0	24.67500
2	0	14.34100
3	0	7.41300
3	0	5.20600
4	0	3.29600
4	0	1.99800
2	1	32.00000
2	1	19.34800
2	1	13.72200
3	1	8.17800
3	1	5.46100
4	1	2.91400
4	1	1.61500
3	2	15.60000
3	2	8.94900
3	2	5.21600
3	2	3.18800

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

1SBR	2SBR	3SBR	4SBR	2PBR	3PBR	4PBR	3DBR
-490.05930	-65.19931	-9.87130	-0.99212	-58.55357	-7.47763	-0.45657	-3.21959
0.94020	-0.29522	0.11733	-0.03600	0.0	0.0	0.0	0.0
0.07695	-0.18979	0.11381	-0.03770	0.0	0.0	0.0	0.0
-0.00920	0.02274	0.06846	-0.02858	0.0	0.0	0.0	0.0
0.00497	1.12765	-0.70697	0.23686	0.0	0.0	0.0	0.0
-0.00149	0.02414	0.86527	-0.33103	0.0	0.0	0.0	0.0
0.00103	-0.00972	0.30744	-0.10721	0.0	0.0	0.0	0.0
-0.00031	0.00210	-0.00342	0.67406	0.0	0.0	0.0	0.0
0.00011	-0.00071	0.00149	0.46137	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.01314	-0.00537	0.00188	0.0
0.0	0.0	0.0	0.0	0.26504	-0.06769	0.01250	0.0
0.0	0.0	0.0	0.0	0.73145	-0.38486	0.10814	0.0
0.0	0.0	0.0	0.0	0.01665	0.52843	-0.17059	0.0
0.0	0.0	0.0	0.0	-0.00278	0.60847	-0.15742	0.0
0.0	0.0	0.0	0.0	0.00049	0.00989	0.59127	0.0
0.0	0.0	0.0	0.0	-0.00019	-0.00069	0.53763	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.04115
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.37105
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.55781
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.13813

ATOM=BR (2P) M

ATOMIC NUMBER= 35

TOTAL ENERGY= -2565.11320

BASIS SET (4,3,1)

	N	L	ZETA
1	1	0	34.24710
2	2	0	12.82170
3	3	0	6.73950
4	4	0	2.63820
2	2	1	15.52820
3	3	1	6.52360
4	4	1	2.25700
3	3	2	6.51970

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

ATOM=BR-(LS)N

ATOMIC NUMBER= 35

TOTAL ENERGY= -2572.53270

BASIS SET (8,7,4)

	N	L	ZETA
1	1	0	36.106000
2	2	0	30.798000
3	3	0	24.525000
4	4	0	20.330000
5	5	0	17.510000
6	6	0	15.336000
7	7	0	13.260000
8	8	0	11.859000
9	9	1	33.295000
10	10	2	19.641000
11	11	2	13.772000
12	12	3	8.064000
13	13	3	5.396000
14	14	3	2.776000
15	15	4	1.391000
16	16	4	18.099000
17	17	2	9.116000
18	18	2	5.270000
19	19	2	3.177000

ORBITALS, ORBITAL ENERGIES, VECTOR COMPONENTS

[illegible]

[illegible]

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